

Supplementary Materials for “Quantum Mechanics/Molecular Mechanics Studies on Mechanistic Photophysics of Sunscreen Oxybenzone in Methanol Solution”

Xue-Ping Chang,^{*a} Li Yu,^a Teng-Shuo Zhang^c and Ganglong Cui^b

a College of Chemistry and Chemical Engineering, Xinyang Normal University, Xinyang 464000, P. R. China

b Key Laboratory of Theoretical and Computational Photochemistry, Ministry of Education, Chemistry College, Beijing Normal University, Beijing 100875, P. R. China

c China College of Chemical Engineering, Zhejiang University of Technology, Hangzhou 310014, P. R. China

E-mail: xuepingchang@xynu.edu.cn

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1. Active Orbitals

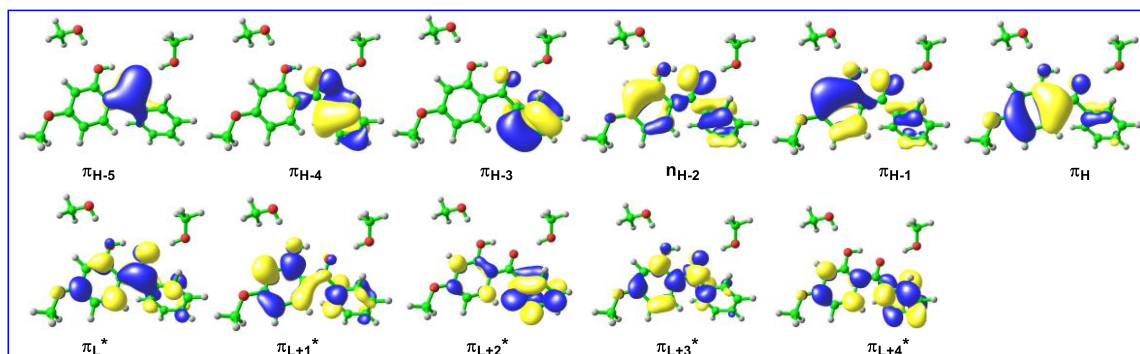


Figure S1. Molecular orbitals (MOs) included in the active space used for QM/MM calculations.

2. Electron Density Differences

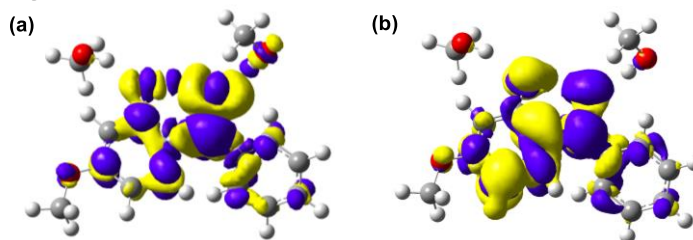


Figure S2. Isosurfaces of electron density differences between (a) the $1n\pi^*$ and S_0 states and (b) the $1\pi\pi^*$ and S_0 states of S0-ENOL computed at TD-CAM-B3LYP/PCM level of theory. Purple (yellow) indicates electron acceptor (donor) regions.

3. Bond-Length Difference of Minima

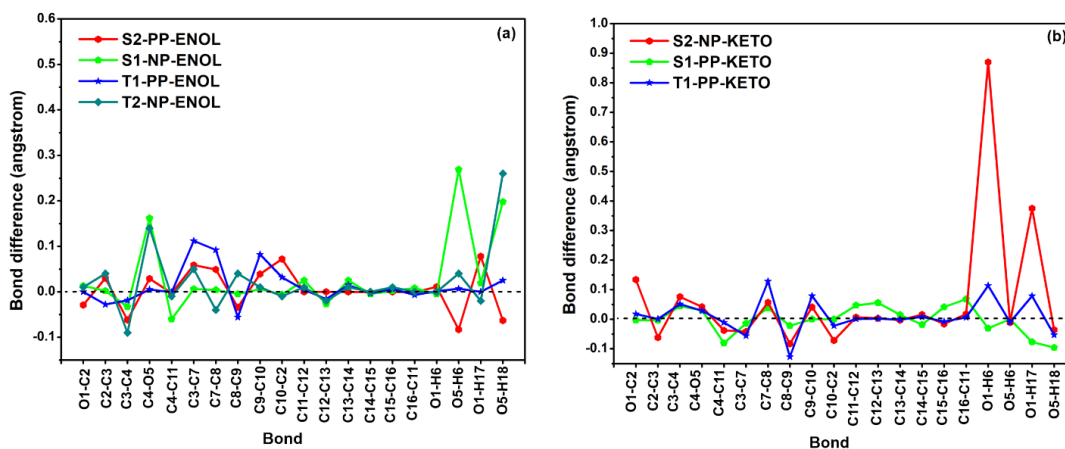


Figure S3. Bond-length difference of (a) the S2-PP-ENOL, S1-NP-ENOL, T2-NP-ENOL, and T1-PP-ENOL minima compared with the counterparts of the S0-ENOL and (b) the S2-NP-KETO, S1-PP-KETO, and T1-PP-KETO minima compared with the counterparts of the S0-KETO. The positive and negative values mean they are longer and shorter than those of the S0-ENOL or S0-KETO, respectively.

4. QM(CASPT2)/MM Computed LIICs

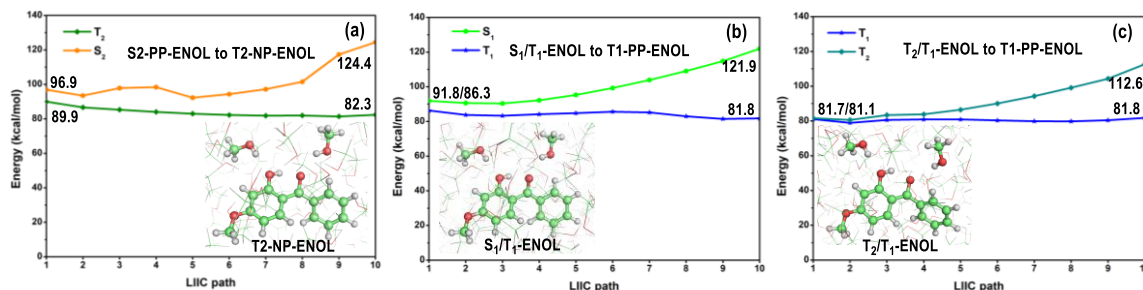


Figure S4. QM(CASPT2)/MM computed linearly interpolated initial coordinate paths (LIICs, in kcal/mol) connecting (a) S₂-PP-ENOL and T₂-NP-ENOL, (b) S₁/T₁-ENOL and T₁-PP-ENOL, and (c) T₂/T₁-ENOL and T₁-PP-ENOL, in methanol solution, respectively.

5. QM(CASPT2)/MM Computed Vertical Excitation Energies and Dipole Moments at the Enol Franck-Condon Point

Table S1: QM(CASPT2)/MM computed vertical excitation energies (in kcal/mol [eV]) and dipole moments (μ , in D) to the lowest four excited-states, i.e., S₁, S₂, T₁, and T₂ at the enol Franck-Condon point, i.e., S₀-ENOL of OB in methanol solution.

	S ₁ (¹ nπ*)	S ₂ (¹ ππ*)	T ₁ (³ ππ*)	T ₂ (³ nπ*)
Energy	93.6 [4.06]	98.9 [4.29]	81.9 [3.55]	82.6 [3.58]
μ	4.97	7.59	6.08	6.06

6. Isomerization Path

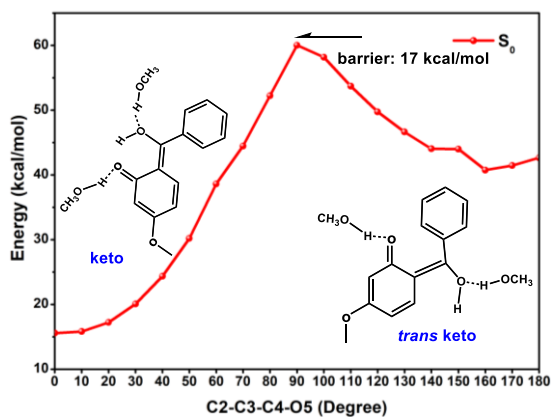


Figure S5. QM(CASPT2//CASSCF)/MM computed S₀ state isomerization path of the solvated OB molecule along the rotation of the central C2-C3-C4-O5 dihedral angle.

7. Cartesian coordinates of All Computed Structures

In xyz format (unit: Ångstrom)

CASSCF/6-31G*

S0-ENOL

C	-2.637431189	-0.695595048	0.436158033
C	-3.736978267	-1.523800110	0.243698019
C	-4.750410342	-1.147863083	-0.635095044
C	-4.675607339	0.053070006	-1.303631095
C	-3.587005259	0.897287067	-1.110708078
C	-2.550899183	0.522000039	-0.253248017
C	-0.005549000	1.052874074	-0.040131003
C	0.369371027	-0.227380018	-0.454634034
C	1.038664077	1.944421139	0.317609020
C	1.693231124	-0.646326048	-0.487964036
C	2.357777168	1.530150110	0.286557021
C	2.689447195	0.231993015	-0.111990009
H	-1.867100136	-0.984384070	1.127377082
H	-3.807979275	-2.453741176	0.776626055
H	-5.595569402	-1.795063131	-0.779434055
H	-5.461169393	0.349656026	-1.973727140
H	-3.548627256	1.843053131	-1.616089115
C	-1.427195105	1.488841106	-0.036476003
O	-1.709663126	2.665927193	0.120122008
H	1.916141140	-1.642602117	-0.814793060
H	3.137568227	2.211928161	0.564997040
O	4.000131287	-0.051352006	-0.099748006
C	4.445979322	-1.319964093	-0.493115037
H	5.520039399	-1.300779094	-0.392400028
H	4.186598299	-1.527752112	-1.525463108
H	4.041023289	-2.096791151	0.146030013
H	-0.383459028	-0.916571064	-0.778715057
O	0.819464060	3.219030233	0.705953052
H	-0.100960008	3.438381246	0.605170044
C	3.567884255	5.470021396	1.689361124
O	2.387378174	5.792071415	1.022001074
H	1.924343139	4.991646359	0.810230059
H	3.390906242	4.822152346	2.545209183
H	4.005295289	6.392334462	2.047926146
H	4.290869311	4.984147356	1.035644073
C	-4.311069308	5.532672400	-0.254039016
O	-4.462977321	4.143584296	-0.278974022
H	-3.659670265	3.729799269	0.007872999

H	-5.254252378	5.967519428	-0.556090040
H	-3.540258255	5.873784420	-0.941803066
H	-4.071159293	5.899610424	0.741088051

S2-PP-ENOL

C	-2.667068194	-0.714328050	0.410641032
C	-3.757864269	-1.547831113	0.192596012
C	-4.769697345	-1.159181084	-0.680955047
C	-4.696870337	0.058379003	-1.319676093
C	-3.613924257	0.904241065	-1.101527080
C	-2.579547188	0.520368035	-0.245603020
C	-0.094308006	1.050139074	-0.028311004
C	0.375477029	-0.266072019	-0.436306033
C	0.984178072	1.973821143	0.259740017
C	1.761616129	-0.649401049	-0.432109033
C	2.381596172	1.569829112	0.227910016
C	2.738523199	0.220639015	-0.116264009
H	-1.900786136	-1.013529073	1.102945079
H	-3.824953276	-2.489420180	0.706164051
H	-5.610683403	-1.807244130	-0.843998061
H	-5.480053395	0.365837028	-1.988014142
H	-3.579336259	1.861877135	-1.584113114
C	-1.454820104	1.473895108	0.000166998
O	-1.739661125	2.673231194	0.204435015
H	1.985899142	-1.660755120	-0.710380049
H	3.136601225	2.291159166	0.463017033
O	4.059871292	-0.012688004	-0.078477007
C	4.534631328	-1.286536093	-0.417397033
H	5.607935401	-1.242371092	-0.318830023
H	4.275798306	-1.541329112	-1.439392106
H	4.142147299	-2.041921148	0.254583020
H	-0.335112024	-0.979014069	-0.795700059
O	0.773445054	3.239391233	0.575941039
H	-0.173157014	3.413760243	0.544947038
C	3.514717255	5.477356396	1.705438121
O	2.377722171	5.864048421	0.996966074
H	1.889982136	5.091735367	0.744862053
H	3.273620238	4.830331347	2.546140181
H	3.980506288	6.373894460	2.091349150
H	4.239245302	4.965677356	1.073222077
C	-4.264641307	5.493194396	-0.229305017
O	-4.444301322	4.109109298	-0.233131016
H	-3.645494263	3.680550266	0.049402004
H	-5.194283372	5.943687428	-0.551544042
H	-3.477735248	5.808620417	-0.911813067
H	-4.030641292	5.873551423	0.762688056

S1-NP-ENOL

C	-2.545250184	-0.782042057	0.261420017
C	-3.680641263	-1.576236115	0.124998011
C	-4.793766347	-1.102078080	-0.555625041
C	-4.771452345	0.194031014	-1.090514081
C	-3.669317262	0.986644070	-0.961577070
C	-2.504846178	0.510357039	-0.301424023
C	0.064005004	0.980752073	-0.116557009
C	0.518421039	-0.285990018	-0.513839036
C	1.054626074	1.885308135	0.352621028
C	1.859994132	-0.654852046	-0.456712034
C	2.384662172	1.529515108	0.391039026
C	2.796089201	0.250946017	-0.017485001
H	-1.705765121	-1.151708085	0.818526061
H	-3.696498266	-2.558752184	0.560308043
H	-5.667693409	-1.716907123	-0.662223046
H	-5.630975403	0.566026041	-1.616744114
H	-3.682103264	1.975556140	-1.378782102
C	-1.339641099	1.348153095	-0.208036013
O	-1.578431115	2.689718192	-0.442020031
H	2.138669153	-1.637289120	-0.783881054
H	3.114399223	2.227306163	0.753184053
O	4.118146296	0.023148001	0.071238005
C	4.629837332	-1.227782088	-0.292166019
H	5.694462412	-1.175303083	-0.123305009
H	4.444196318	-1.442855105	-1.339113096
H	4.210285305	-2.019571146	0.319160023
H	-0.183955014	-0.988200073	-0.915301065
O	0.761654054	3.150103224	0.768008054
H	-0.147436010	3.247820233	1.015736071
C	3.378310241	5.632120405	1.623142116
O	2.127133153	5.852770421	1.047896077
H	1.741305126	5.018526362	0.813450061
H	3.323218238	4.963406360	2.479633179
H	3.755633268	6.587486474	1.963152141
H	4.091381294	5.219862377	0.911312063
C	-4.420860321	5.961699431	-0.604660044
O	-4.138316299	4.610204333	-0.375253028
H	-3.201185228	4.484727321	-0.331363025
H	-5.496695395	6.068141439	-0.608186042
H	-4.037447289	6.301702454	-1.563657111
H	-4.017269290	6.600492476	0.176879014

T2-NP-ENOL

C	-2.681157195	-0.782588057	0.402199030
C	-3.810428276	-1.561298113	0.145473011
C	-4.796031343	-1.096028076	-0.716977053

C	-4.653830335	0.150588012	-1.317709094
C	-3.540105254	0.918656065	-1.073146076
C	-2.525517180	0.459548032	-0.218119014
C	0.000629001	1.019296073	-0.006519998
C	0.435151030	-0.320303025	-0.350518024
C	1.077250079	1.966075141	0.239616020
C	1.733753126	-0.682882052	-0.409203030
C	2.394200174	1.579338115	0.179370010
C	2.755256197	0.258267020	-0.129515010
H	-1.938832139	-1.133594083	1.095291081
H	-3.922086284	-2.515419182	0.627458043
H	-5.668583406	-1.691918124	-0.908322064
H	-5.416328389	0.518859039	-1.979137141
H	-3.453206248	1.884642134	-1.535648109
C	-1.362595099	1.338241097	0.054113004
O	-1.716114124	2.603779188	0.414091029
H	1.978754144	-1.690383124	-0.685161049
H	3.164370229	2.303532166	0.363089027
O	4.073254295	-0.008716999	-0.146101012
C	4.525313327	-1.297450093	-0.454264034
H	5.601710404	-1.258297089	-0.388351028
H	4.241243306	-1.589323113	-1.459809103
H	4.153067300	-2.029785145	0.254147021
H	-0.311593021	-1.045286074	-0.599393043
O	0.851550061	3.273152233	0.538261037
H	-0.056050004	3.509995253	0.403730030
C	3.476136249	5.635564407	1.706892121
O	2.323109168	5.869112420	0.958807071
H	1.929676139	5.037074363	0.728756052
H	3.283376234	4.998744361	2.567500182
H	3.834549275	6.591427474	2.065821147
H	4.266514309	5.178814373	1.113109082
C	-4.217479306	5.544240400	-0.278316022
O	-4.529164324	4.182285298	-0.196332014
H	-3.921287284	3.752046272	0.388764030
H	-4.956558356	6.005292433	-0.918524067
H	-3.234045230	5.713035411	-0.711356053
H	-4.255782308	6.030295434	0.693171051

T1-PP-ENOL

C	-2.578486188	-0.735807053	0.390876029
C	-3.664826262	-1.583054114	0.168210011
C	-4.704628340	-1.179017087	-0.660382049
C	-4.668483337	0.078489004	-1.256158091
C	-3.611395261	0.926666067	-1.023365076
C	-2.547440184	0.524556039	-0.206564016
C	-0.033370002	1.089458076	-0.026326002

C	0.351649024	-0.275816019	-0.541001037
C	1.005283074	1.986073141	0.199334016
C	1.743178127	-0.749114056	-0.360360028
C	2.353191170	1.565669112	0.104642007
C	2.690949196	0.139226010	-0.102580010
H	-1.777685130	-1.052686078	1.033468075
H	-3.698261268	-2.548139185	0.638848048
H	-5.537050399	-1.835154134	-0.834141060
H	-5.472475392	0.393670026	-1.895383136
H	-3.605607258	1.906053138	-1.462526105
C	-1.440857101	1.499104107	0.050867004
O	-1.738941127	2.665981190	0.277831021
H	1.945814140	-1.792959128	-0.502702035
H	3.148413228	2.270417164	0.237104015
O	4.006073291	-0.072519006	0.031629004
C	4.503075325	-1.369144101	-0.158121009
H	5.571480402	-1.306192096	-0.020529003
H	4.285357311	-1.725813123	-1.158858085
H	4.085593296	-2.056856149	0.568679039
H	-0.150002012	-0.594185044	-1.437738104
O	0.831180060	3.276348236	0.555861038
H	-0.098118008	3.486479251	0.556524039
C	3.471170249	5.543593401	1.720880122
O	2.359988171	5.859396424	0.940463068
H	1.917111138	5.057327363	0.695296052
H	3.209706231	4.916922356	2.570750182
H	3.883127281	6.470683466	2.096949152
H	4.246486305	5.037338364	1.147316083
C	-4.298659308	5.563532403	-0.249057018
O	-4.477743324	4.178010303	-0.207614015
H	-3.695704267	3.764223270	0.133435012
H	-5.220090378	5.998552430	-0.611517044
H	-3.494331252	5.853720421	-0.921711068
H	-4.091298292	5.978250428	0.734430054

S0-KETO

C	-2.611519188	-0.702909050	0.416026030
C	-3.722309267	-1.494049109	0.177638013
C	-4.717291340	-1.066234074	-0.680956047
C	-4.610116330	0.174598012	-1.303421096
C	-3.500459252	0.977342070	-1.068714079
C	-2.479381179	0.536197039	-0.217655016
C	0.011367002	1.067394078	-0.025149001
C	0.430194031	-0.263202021	-0.412811029
C	1.069974077	2.056642150	0.269899019
C	1.707696121	-0.627418047	-0.452347031
C	2.449073177	1.602946114	0.237246015

C	2.762397200	0.326607023	-0.102378007
H	-1.861971133	-1.034032072	1.111184078
H	-3.815631273	-2.442894175	0.673873047
H	-5.578295400	-1.684541124	-0.855018061
H	-5.384957386	0.519255038	-1.962581143
H	-3.432964249	1.941186141	-1.534327113
C	-1.317771092	1.427928105	0.023350999
O	-1.702131123	2.677761194	0.278511019
H	1.967895141	-1.619117115	-0.764833054
H	3.219111229	2.310687166	0.475157036
O	4.064676295	-0.010627001	-0.116938007
C	4.478374320	-1.315829096	-0.418769030
H	5.552343400	-1.312456094	-0.314319025
H	4.224321303	-1.592607112	-1.435949104
H	4.060354293	-2.039750145	0.271593021
H	-0.319766021	-0.969083069	-0.706132052
O	0.813908058	3.230410232	0.539201041
H	-0.932742065	3.234980234	0.413852032
C	3.407998244	5.554712399	1.730660122
O	2.266502163	5.865824420	0.994396072
H	1.813629130	5.062804363	0.770384055
H	3.183386230	4.924698356	2.588815188
H	3.828472278	6.483168467	2.094007149
H	4.164198300	5.054511362	1.127197082
C	-4.269606307	5.545711401	-0.280331018
O	-4.454673318	4.160483302	-0.263649017
H	-3.685316264	3.738294267	0.095327006
H	-5.171266374	5.988058432	-0.681470048
H	-3.433295245	5.840904420	-0.910528066
H	-4.108574294	5.948627430	0.716704050

S2-NP-KETO

C	-2.556504186	-0.709253049	0.285683021
C	-3.654823261	-1.515992111	0.170116013
C	-4.773118343	-1.104817081	-0.561980042
C	-4.770060344	0.149798009	-1.158740084
C	-3.660625261	0.984370073	-1.042254074
C	-2.516737182	0.561836042	-0.337552023
C	0.032354003	1.008480071	-0.135956007
C	0.483778037	-0.263156020	-0.529840038
C	1.044043074	1.890452135	0.318581024
C	1.812619131	-0.649261045	-0.458950030
C	2.375269170	1.529763112	0.377839028
C	2.765403197	0.245331018	-0.010814002
H	-1.723718126	-1.035983075	0.879973065
H	-3.665804266	-2.474259177	0.657295046
H	-5.627765403	-1.749497128	-0.647594047

H	-5.622884405	0.482591035	-1.721080125
H	-3.678552262	1.951851143	-1.502692108
C	-1.356914095	1.422165100	-0.255724017
O	-1.590419113	2.766000199	-0.419165030
H	2.081637149	-1.635935119	-0.781162057
H	3.117712227	2.222343157	0.725030051
O	4.084247297	-0.004940002	0.080436005
C	4.579869331	-1.259516091	-0.294417023
H	5.645303406	-1.221381086	-0.126693008
H	4.390487314	-1.463888107	-1.342871096
H	4.152065298	-2.051125149	0.311024023
H	-0.226300015	-0.958368071	-0.930864067
O	0.735429051	3.154083225	0.733991054
H	-1.090065080	3.114565226	-1.146707085
C	3.291122235	5.625018407	1.543939109
O	2.052108149	6.195105444	1.241245087
H	1.427526105	5.508461398	1.053291076
H	3.226947233	4.922317355	2.371761169
H	3.954340283	6.428646462	1.833258134
H	3.727517266	5.115268366	0.687152052
C	-4.318231309	5.722307411	-0.255362017
O	-4.209594305	4.390597314	-0.660715049
H	-3.434083248	3.994525289	-0.284704022
H	-5.252948380	6.105300440	-0.641119044
H	-3.509587252	6.337775457	-0.645169044
H	-4.332387314	5.819461417	0.827200059

S1-PP-KETO

C	-2.635786188	-0.672508050	0.206697014
C	-3.774533273	-1.510265111	0.024553004
C	-4.920704354	-1.053976075	-0.558274039
C	-4.997388361	0.296223020	-0.945500068
C	-3.877278280	1.194591086	-0.770671054
C	-2.598325186	0.699614049	-0.306705022
C	-0.117274008	1.148232084	-0.142768011
C	0.331478026	-0.191503013	-0.389666028
C	0.924319066	2.154810155	0.134237012
C	1.644304121	-0.562960041	-0.305476023
C	2.298672165	1.703757121	0.264803021
C	2.648913192	0.410289029	0.047887001
H	-1.836832134	-1.028998073	0.823261060
H	-3.720110266	-2.520688184	0.384840027
H	-5.765215415	-1.701971121	-0.691515049
H	-5.896692424	0.685371047	-1.380154099
H	-4.007025286	2.229213159	-1.000284074
C	-1.479189108	1.544761112	-0.260761017
O	-1.784070130	2.865855205	-0.394693027

H	1.919123138	-1.571076113	-0.542699040
H	3.038310218	2.443452177	0.503044037
O	3.955194285	0.093156008	0.164223010
C	4.399741317	-1.216021087	-0.054307006
H	5.462319396	-1.201911089	0.135099010
H	4.228593303	-1.533498109	-1.077625075
H	3.932161284	-1.920182139	0.625678044
H	-0.372779024	-0.925755067	-0.720476052
O	0.658249046	3.346554240	0.262067021
H	-0.987026072	3.376814241	-0.237622016
C	2.656111193	6.005083435	1.829757129
O	2.923659210	5.194923375	0.727122053
H	2.142245153	4.699605336	0.505378037
H	1.914941135	6.770430490	1.605878116
H	3.577790257	6.499892468	2.107922151
H	2.305170166	5.431832388	2.685268193
C	-4.244869303	5.779828417	-0.693238050
O	-4.353598315	4.523321324	-0.089960005
H	-3.493088252	4.129923300	-0.009919999
H	-5.244085375	6.184853445	-0.781812056
H	-3.808767273	5.720562412	-1.687925122
H	-3.651505261	6.468444464	-0.096766008

T1-PP-KETO

C	-2.644569192	-0.728275051	0.387187028
C	-3.731929270	-1.539068112	0.153002013
C	-4.757312343	-1.121638080	-0.687622051
C	-4.685233337	0.131623009	-1.286621095
C	-3.588897259	0.956337067	-1.053740078
C	-2.542022182	0.531436037	-0.223420016
C	-0.024544003	1.053438076	-0.028619001
C	0.407289027	-0.223071018	-0.378902028
C	1.053265078	2.024341144	0.263039019
C	1.806889131	-0.627978044	-0.403566027
C	2.415889175	1.594235116	0.219114016
C	2.778613202	0.245426016	-0.114776011
H	-1.879779133	-1.054533076	1.068138075
H	-3.796532272	-2.497316182	0.636248047
H	-5.604355401	-1.758799128	-0.859599063
H	-5.475024396	0.469498036	-1.931817138
H	-3.549549258	1.926971139	-1.507620109
C	-1.401666102	1.430838104	0.021825000
O	-1.782582126	2.731372194	0.146876008
H	2.019257148	-1.646301119	-0.664962046
H	3.181782230	2.311863168	0.437956029
O	4.103368296	0.022504003	-0.090893008
C	4.578089327	-1.258793092	-0.399694027

H	5.652243407	-1.209961086	-0.312042023
H	4.310949312	-1.542177113	-1.412130100
H	4.193362301	-1.996792145	0.295919024
H	-0.309556022	-0.960684068	-0.673054050
O	0.821174059	3.221138232	0.535095038
H	-1.028187071	3.287926238	0.300659023
C	3.429554247	5.558772401	1.737109126
O	2.278880164	5.929631427	1.042281072
H	1.801987130	5.150099368	0.792734057
H	3.208504231	4.900366353	2.574527185
H	3.881163277	6.460897465	2.126710155
H	4.157675297	5.066121362	1.094222079
C	-4.298487309	5.548618399	-0.269717019
O	-4.535530327	4.174030303	-0.213512013
H	-3.747636267	3.723205270	0.062874004
H	-5.213506376	6.023369435	-0.597957041
H	-3.509881253	5.802358419	-0.975643073
H	-4.034928289	5.959594427	0.702422048

S₁/T₁-ENOL

C	-2.469552178	-0.786661055	0.212133014
C	-3.585748257	-1.587487116	0.103219007
C	-4.770590342	-1.103014079	-0.489884034
C	-4.825860350	0.271153021	-0.904117063
C	-3.769465273	1.083573080	-0.784134054
C	-2.486341178	0.581915043	-0.280710020
C	0.068000007	0.956758070	-0.161327013
C	0.552811040	-0.272376018	-0.598701043
C	1.014688072	1.851853132	0.391392030
C	1.897346135	-0.633466046	-0.491354035
C	2.345777169	1.511574110	0.489077033
C	2.795050199	0.260839017	0.040509005
H	-1.588874116	-1.163384085	0.693201050
H	-3.557207257	-2.593452188	0.479232034
H	-5.633900404	-1.732291126	-0.579618043
H	-5.748039412	0.653934045	-1.299760095
H	-3.851235276	2.115423153	-1.059855075
C	-1.342683096	1.376446102	-0.387819030
O	-1.492456106	2.583363186	-0.921179065
H	2.205914156	-1.595344112	-0.851445061
H	3.048457218	2.203529160	0.911781068
O	4.114647296	0.044318002	0.181438014
C	4.661612336	-1.177021083	-0.228686017
H	5.718691411	-1.117220080	-0.018394000
H	4.517371323	-1.338533097	-1.291800094
H	4.233993303	-2.007052146	0.323815026
H	-0.119393008	-0.965811071	-1.064656078

O	0.675202049	3.094318221	0.833918060
H	-0.256870019	3.184900227	0.974107072
C	3.308343240	5.634694408	1.597541113
O	2.047976148	5.830402422	1.032983074
H	1.659228120	4.987066361	0.838821062
H	3.269335236	4.989260357	2.472645176
H	3.682194266	6.602018475	1.906717139
H	4.015083290	5.208555372	0.887559064
C	-4.360151313	5.942669428	-0.684713047
O	-4.092620293	4.600604332	-0.387243026
H	-3.180290231	4.407835316	-0.560427039
H	-5.417771392	6.101358440	-0.516746039
H	-4.134837298	6.185255445	-1.722292126
H	-3.803863276	6.620969477	-0.040054003

T_2/T_1 -ENOL

C	-2.683791195	-0.781605058	0.403071030
C	-3.813570276	-1.559124110	0.145827010
C	-4.799407345	-1.092733080	-0.716119050
C	-4.656507337	0.153805013	-1.316550095
C	-3.541633253	0.920594065	-1.072640077
C	-2.526750184	0.460127032	-0.218244017
C	0.006216002	1.014620073	-0.006567000
C	0.439881033	-0.321357024	-0.350373024
C	1.077987080	1.961067140	0.239376017
C	1.740970125	-0.683515048	-0.409317030
C	2.396794174	1.576610116	0.179299011
C	2.759468199	0.257549017	-0.129850011
H	-1.941982140	-1.132823083	1.096505077
H	-3.925580282	-2.513477181	0.627143045
H	-5.672494406	-1.687855123	-0.907175067
H	-5.419065389	0.523036036	-1.977303145
H	-3.453813251	1.886357134	-1.535305112
C	-1.359963098	1.332242095	0.054079004
O	-1.716509123	2.597789187	0.416860029
H	1.986957142	-1.690733122	-0.685388050
H	3.165684229	2.302097165	0.363591025
O	4.078188291	-0.007246003	-0.146634010
C	4.531317324	-1.295421095	-0.455058032
H	5.607715401	-1.255300088	-0.389331027
H	4.246685307	-1.587366115	-1.460483105
H	4.159207302	-2.028082147	0.253178018
H	-0.306044021	-1.047181074	-0.599667045
O	0.851085062	3.268732233	0.538732036
H	-0.054729003	3.509170250	0.401868030
C	3.473057253	5.636176406	1.707037120
O	2.319832170	5.866365424	0.958157067

H	1.929108136	5.033091362	0.727859054
H	3.281224234	4.999150362	2.567700185
H	3.828409274	6.593256475	2.065742147
H	4.264870309	5.181371373	1.113714080
C	-4.220039301	5.553875400	-0.283279022
O	-4.535386327	4.192818302	-0.198099017
H	-3.934820283	3.764874269	0.395989029
H	-4.953225355	6.013264430	-0.931204069
H	-3.233064231	5.718484413	-0.709478050
H	-4.264957305	6.043962436	0.685794050

T₁/S₀-ENOL

C	-2.495403179	-0.784348058	0.383046026
C	-3.555586255	-1.662881121	0.156119010
C	-4.655586335	-1.247907090	-0.586536041
C	-4.704632340	0.051733003	-1.090059079
C	-3.677123267	0.930044065	-0.846250059
C	-2.555387183	0.517088036	-0.114793008
C	-0.063991002	1.152610084	-0.117662011
C	0.399085028	-0.036183002	-0.915823067
C	1.004707075	2.031166144	0.085667007
C	1.599824116	-0.760871057	-0.391817028
C	2.314765165	1.533206109	-0.030784003
C	2.589171186	0.081224003	-0.105440006
H	-1.642773116	-1.107157081	0.954657067
H	-3.525374255	-2.659514189	0.555286040
H	-5.467262393	-1.927478138	-0.767370057
H	-5.553908399	0.371533029	-1.665260122
H	-3.736418271	1.937859140	-1.211194085
C	-1.462696103	1.502445110	0.146326008
O	-1.746886125	2.646054190	0.471765037
H	1.682192122	-1.828356133	-0.409442027
H	3.147376226	2.193654157	0.121930011
O	3.871148280	-0.190908011	0.179007011
C	4.321430313	-1.510325109	0.040256000
H	5.377397385	-1.494890110	0.263361018
H	4.164680302	-1.867262133	-0.972053071
H	3.818590274	-2.172976159	0.735294052
H	0.553923038	0.260413019	-1.948816142
O	0.871722064	3.316845240	0.476744033
H	-0.054130006	3.523860253	0.569829042
C	3.292251235	5.700649409	1.798847129
O	2.360778169	5.916639427	0.783921055
H	1.958977139	5.089335368	0.551586037
H	2.853114204	5.195245374	2.656301189
H	3.654536262	6.667422481	2.123015154
H	4.145453297	5.116762366	1.456597103

C	-4.257737306	5.583869404	-0.214528018
O	-4.457376319	4.208210300	-0.064509003
H	-3.689251263	3.811854276	0.325671025
H	-5.160731370	5.996285429	-0.643507047
H	-3.427552248	5.807939419	-0.880968061
H	-4.078156292	6.076420438	0.737935054

S₁/S₀-KETO

C	-2.361268172	-0.412923029	0.274232017
C	-3.525952255	-1.149798083	0.446358030
C	-4.719454341	-0.717282049	-0.123326007
C	-4.745104340	0.473842036	-0.850902062
C	-3.607147259	1.214351088	-1.024448074
C	-2.375631169	0.773464057	-0.487865037
C	0.183669015	0.880614063	-0.566764042
C	0.735520053	-0.264527018	-1.090559077
C	0.940522065	1.690681120	0.295938021
C	2.089636150	-0.590853043	-0.775326057
C	2.254332160	1.358531097	0.643119049
C	2.820380204	0.213160015	0.058832006
H	-1.444344104	-0.759299056	0.712433050
H	-3.501715254	-2.064002148	1.009193074
H	-5.615637401	-1.296207093	-0.001730002
H	-5.666343409	0.809073056	-1.289450092
H	-3.643936265	2.125836155	-1.585730115
C	-1.161100082	1.483672107	-0.760630054
O	-1.277463090	2.511836181	-1.635604119
H	2.507892180	-1.485787107	-1.194535088
H	2.823368204	1.948036140	1.334578095
O	4.101608295	-0.016888999	0.416629032
C	4.741155339	-1.181164086	-0.019295004
H	5.732596411	-1.156883084	0.406567029
H	4.820733347	-1.210210085	-1.100972079
H	4.225577305	-2.070395149	0.327959024
H	0.164512010	-0.921835065	-1.717998122
O	0.288168022	2.751130196	0.701835048
H	-0.485222035	3.029184217	-1.634029118
C	3.067683222	5.352814387	1.372228099
O	1.739038125	5.627416405	1.040245074
H	1.216120085	4.843053350	1.143235084
H	3.166642225	4.977625358	2.388343171
H	3.618180261	6.280996452	1.299226091
H	3.520353252	4.633827334	0.692455048
C	-4.325777313	6.012000432	-0.719186050
O	-4.156506302	4.641234334	-0.498944035
H	-3.236468232	4.419956317	-0.541970040
H	-5.383221388	6.221117448	-0.633618047

H	-3.995207287	6.310935454	-1.711337125
H	-3.799327275	6.612594474	0.017817001

T₁/S₀-KETO

C	-2.587998186	-0.590960042	0.332717026
C	-3.639730263	-1.452526105	0.343815026
C	-4.823980347	-1.156304085	-0.355040024
C	-4.921975353	0.045266002	-1.041327077
C	-3.857878277	0.947642066	-1.048952077
C	-2.653758191	0.641994044	-0.379545026
C	-0.107633007	1.098730077	-0.285974021
C	0.386298026	-0.031917003	-0.837489059
C	0.837778059	1.985693144	0.388810026
C	1.784094128	-0.454196034	-0.688140052
C	2.192360160	1.573430115	0.527966036
C	2.650684189	0.323067023	-0.030117001
H	-1.697698121	-0.839067060	0.879797066
H	-3.570290259	-2.374280169	0.892125065
H	-5.641459404	-1.852586132	-0.347591023
H	-5.820845417	0.283978023	-1.579468112
H	-3.950017286	1.871328135	-1.582938113
C	-1.541429111	1.540555111	-0.414681030
O	-1.721796123	2.715771197	-1.097087076
H	2.070795149	-1.397205101	-1.109886080
H	2.885694208	2.204798159	1.047951074
O	3.950085285	0.084116005	0.195062015
C	4.510251323	-1.113295082	-0.273703020
H	5.546573399	-1.097543079	0.025960002
H	4.447123319	-1.176253083	-1.354439096
H	4.019093290	-1.972554144	0.169211014
H	-0.267275019	-0.692901049	-1.373826097
O	0.482637036	3.123937225	0.770030057
H	-1.109442079	3.355967240	-0.751548054
C	3.295239234	5.489293396	1.362540096
O	1.943695140	5.831201421	1.368208098
H	1.419580101	5.042773364	1.310497096
H	3.562500257	4.850640350	2.202868159
H	3.862678279	6.406412460	1.443278103
H	3.589487260	4.988850361	0.441203034
C	-4.275253306	5.761686417	-0.811152061
O	-4.370696313	4.443316317	-0.359280025
H	-3.573729255	3.971995287	-0.564273041
H	-5.204299374	6.256419450	-0.560900039
H	-4.137820296	5.818736418	-1.889043137
H	-3.463238247	6.303387455	-0.331540024

S₂ state minimum-energy proton transfer path

1.8 angstrom

C	-2.667068194	-0.714328050	0.410641032
C	-3.757864269	-1.547831113	0.192596012
C	-4.769697345	-1.159181084	-0.680955047
C	-4.696870337	0.058379003	-1.319676093
C	-3.613924257	0.904241065	-1.101527080
C	-2.579547188	0.520368035	-0.245603020
C	-0.094308006	1.050139074	-0.028311004
C	0.375477029	-0.266072019	-0.436306033
C	0.984178072	1.973821143	0.259740017
C	1.761616129	-0.649401049	-0.432109033
C	2.381596172	1.569829112	0.227910016
C	2.738523199	0.220639015	-0.116264009
H	-1.900786136	-1.013529073	1.102945079
H	-3.824953276	-2.489420180	0.706164051
H	-5.610683403	-1.807244130	-0.843998061
H	-5.480053395	0.365837028	-1.988014142
H	-3.579336259	1.861877135	-1.584113114
C	-1.454820104	1.473895108	0.000166998
O	-1.739661125	2.673231194	0.204435015
H	1.985899142	-1.660755120	-0.710380049
H	3.136601225	2.291159166	0.463017033
O	4.059871292	-0.012688004	-0.078477007
C	4.534631328	-1.286536093	-0.417397033
H	5.607935401	-1.242371092	-0.318830023
H	4.275798306	-1.541329112	-1.439392106
H	4.142147299	-2.041921148	0.254583020
H	-0.335112024	-0.979014069	-0.795700059
O	0.773445054	3.239391233	0.575941039
H	-0.173157014	3.413760243	0.544947038
C	3.514717255	5.477356396	1.705438121
O	2.377722171	5.864048421	0.996966074
H	1.889982136	5.091735367	0.744862053
H	3.273620238	4.830331347	2.546140181
H	3.980506288	6.373894460	2.091349150
H	4.239245302	4.965677356	1.073222077
C	-4.264641307	5.493194396	-0.229305017
O	-4.444301322	4.109109298	-0.233131016
H	-3.645494263	3.680550266	0.049402004
H	-5.194283372	5.943687428	-0.551544042
H	-3.477735248	5.808620417	-0.911813067
H	-4.030641292	5.873551423	0.762688056

1.7 angstrom

C	-2.668599194	-0.712227052	0.411737032
C	-3.761588269	-1.542676112	0.193462016
C	-4.773056345	-1.150059084	-0.678839047

C	-4.697405340	0.068216006	-1.315907097
C	-3.612115260	0.911080067	-1.097505079
C	-2.578218186	0.523089038	-0.242996018
C	-0.091406009	1.039915073	-0.028831000
C	0.382305030	-0.272213021	-0.435656029
C	0.980775071	1.969747139	0.258188019
C	1.771991130	-0.649281048	-0.428610029
C	2.379981170	1.574523115	0.231060018
C	2.743908197	0.225368018	-0.111451010
H	-1.902627138	-1.013601073	1.103464080
H	-3.830639275	-2.484956178	0.705568050
H	-5.615801404	-1.795709130	-0.842490059
H	-5.480225394	0.378754028	-1.983226141
H	-3.575319258	1.869219136	-1.578917112
C	-1.448537104	1.469125104	0.002341001
O	-1.722933123	2.672674192	0.209104014
H	2.001645145	-1.659807120	-0.705588052
H	3.131042223	2.300605165	0.464955033
O	4.066216291	-0.001433001	-0.070954006
C	4.547622328	-1.274345093	-0.404712029
H	5.620587405	-1.225367087	-0.303262020
H	4.292886307	-1.533319109	-1.426776102
H	4.156421300	-2.029455145	0.268408020
H	-0.324619021	-0.989628074	-0.794313059
O	0.749029054	3.231316232	0.561006038
H	-0.207625017	3.378143243	0.519226039
C	3.490464252	5.466201392	1.706749121
O	2.363622169	5.856312421	0.984283071
H	1.863524136	5.087477369	0.745417054
H	3.234808235	4.840153348	2.559079184
H	3.968604287	6.362931458	2.077036149
H	4.210450302	4.930499356	1.089159080
C	-4.257081306	5.493524396	-0.231041015
O	-4.431274317	4.108648294	-0.235622018
H	-3.632064263	3.683120263	0.050396005
H	-5.186690372	5.940188428	-0.558475042
H	-3.467676250	5.811856421	-0.909251066
H	-4.030004290	5.874813421	0.762157053

1.6 angstrom

C	-2.669489191	-0.711044050	0.408761029
C	-3.764748272	-1.537557110	0.188108013
C	-4.775945346	-1.138317080	-0.681699049
C	-4.697289339	0.082572008	-1.313365094
C	-3.609609261	0.921650065	-1.092267076
C	-2.575875185	0.526782039	-0.240788015
C	-0.086829006	1.023440071	-0.030530003

C	0.392268030	-0.282350020	-0.432024031
C	0.976121068	1.962959139	0.253053016
C	1.786350127	-0.650567049	-0.421685030
C	2.377055169	1.580704112	0.230089014
C	2.751229200	0.231681018	-0.106758007
H	-1.904009138	-1.016937075	1.099049080
H	-3.835881278	-2.481766181	0.696470048
H	-5.620642402	-1.780832126	-0.847609061
H	-5.479549396	0.398015027	-1.979006143
H	-3.570287259	1.881565138	-1.569822111
C	-1.438854102	1.461532104	0.003267998
O	-1.696998120	2.671921194	0.212711013
H	2.023206144	-1.660641119	-0.693946052
H	3.122520226	2.313800168	0.460048031
O	4.074851294	0.014768003	-0.062941003
C	4.565563326	-1.256812090	-0.388822027
H	5.637962405	-1.200183087	-0.285616022
H	4.314496313	-1.522871108	-1.409941101
H	4.177950300	-2.010693144	0.287715020
H	-0.309359020	-1.006414074	-0.788370054
O	0.713593049	3.215723230	0.540699041
H	-0.260511017	3.320654237	0.487783036
C	3.463875249	5.445913393	1.705525123
O	2.346340171	5.843801422	0.973182070
H	1.830363132	5.081242364	0.747641054
H	3.194933232	4.839895347	2.568204184
H	3.957734283	6.340144456	2.061071147
H	4.175791299	4.886425353	1.099596080
C	-4.247246304	5.498348397	-0.229915016
O	-4.408169317	4.111838297	-0.233634015
H	-3.605463258	3.693740268	0.053862005
H	-5.180244374	5.935743429	-0.560272043
H	-3.459082248	5.823577422	-0.906252065
H	-4.026510291	5.882654426	0.763522055

1.5 angstrom

C	-2.669432193	-0.712091053	0.404403027
C	-3.766740270	-1.534522109	0.180657012
C	-4.778376344	-1.127639083	-0.685481047
C	-4.697175338	0.096862006	-1.309716094
C	-3.607258259	0.931801066	-1.085010077
C	-2.572988184	0.529249037	-0.237730016
C	-0.081935006	1.006974070	-0.031645001
C	0.402340030	-0.291043021	-0.425825032
C	0.971808072	1.957305140	0.247152017
C	1.800958129	-0.651924045	-0.413716028
C	2.373705171	1.586514113	0.228829017

C	2.758769198	0.237742018	-0.102204008
H	-1.904450138	-1.023440071	1.092777081
H	-3.839524277	-2.481392180	0.683948047
H	-5.624986402	-1.766926126	-0.854097059
H	-5.479106396	0.418076030	-1.972956144
H	-3.565765254	1.894147136	-1.557270111
C	-1.429109102	1.452561105	0.004165001
O	-1.671955119	2.671524195	0.213890015
H	2.043850147	-1.661928120	-0.680496050
H	3.113548226	2.326606168	0.454667034
O	4.083536294	0.031361002	-0.055317004
C	4.583726330	-1.238822091	-0.373289029
H	5.655530407	-1.174158086	-0.269062019
H	4.335744314	-1.512182109	-1.393186100
H	4.200270303	-1.991274144	0.307142021
H	-0.294288020	-1.022805074	-0.776861058
O	0.681576047	3.199260230	0.517113040
H	-0.315395022	3.264291234	0.455520031
C	3.440574247	5.425402393	1.705334122
O	2.331790168	5.829649418	0.963528068
H	1.802596128	5.073033365	0.748168056
H	3.159987229	4.835403347	2.575365185
H	3.946550286	6.317036455	2.050308147
H	4.146612296	4.847428350	1.109845079
C	-4.233857304	5.502410399	-0.231285018
O	-4.381868313	4.114529295	-0.232493019
H	-3.575088257	3.703767267	0.054804004
H	-5.170453372	5.930465426	-0.563824039
H	-3.447770248	5.833671419	-0.907099066
H	-4.018161287	5.890727421	0.761692054

1.4 angstrom

C	-2.660478191	-0.735390050	0.390295029
C	-3.760390270	-1.548644109	0.152848012
C	-4.775321345	-1.119604082	-0.701041049
C	-4.691538336	0.118412009	-1.297777093
C	-3.598708258	0.942625069	-1.058971074
C	-2.561664183	0.518952036	-0.224254015
C	-0.064349007	0.987880069	-0.022991000
C	0.428835029	-0.301853022	-0.389484028
C	0.974366073	1.961552142	0.233110018
C	1.831937133	-0.647353049	-0.382309025
C	2.374313169	1.608351115	0.219809016
C	2.778523200	0.260859020	-0.089987004
H	-1.897232134	-1.062811075	1.072933077
H	-3.835289277	-2.505526181	0.636650047
H	-5.624607406	-1.752352124	-0.880372065

H	-5.473793393	0.456898035	-1.951984141
H	-3.554325257	1.913616139	-1.512347111
C	-1.411916101	1.428016102	0.018434001
O	-1.647234117	2.663061190	0.220511017
H	2.085144150	-1.659328119	-0.630984046
H	3.105567223	2.363856171	0.422003028
O	4.105364295	0.073019004	-0.043049003
C	4.621338333	-1.198621088	-0.329793025
H	5.692096407	-1.118287081	-0.227034016
H	4.377092314	-1.499768108	-1.342674094
H	4.246501307	-1.938568137	0.368854027
H	-0.261168017	-1.054815075	-0.707772052
O	0.653798047	3.194339230	0.464524034
H	-0.375387027	3.216762233	0.409777028
C	3.356522241	5.433495391	1.743363128
O	2.301107164	5.823813419	0.921086068
H	1.766430128	5.069136366	0.712199053
H	3.013521217	4.891594351	2.622082191
H	3.862803276	6.330239454	2.074605151
H	4.081648295	4.813304344	1.217434085
C	-4.187626300	5.525272396	-0.269813017
O	-4.323308310	4.136238300	-0.265578017
H	-3.519443253	3.732719269	0.040033005
H	-5.116444367	5.942325426	-0.636257043
H	-3.382742243	5.858835422	-0.921911066
H	-4.008799289	5.922636429	0.726925051

1.3 angstrom

C	-2.668616191	-0.649298045	0.276233022
C	-3.837182276	-1.432457106	0.080259006
C	-4.930759357	-0.938144070	-0.664586050
C	-4.866104348	0.371951026	-1.190726086
C	-3.717358269	1.174059082	-0.980210068
C	-2.578053183	0.664061048	-0.278043020
C	-0.059623004	1.089916079	-0.063609005
C	0.386646029	-0.217652015	-0.329245025
C	0.953624071	2.094054151	0.195396016
C	1.754783127	-0.557174038	-0.284440021
C	2.292945166	1.756801129	0.261257020
C	2.701729193	0.432199030	0.023621001
H	-1.887925134	-1.027602077	0.904799066
H	-3.887475282	-2.411157172	0.518767036
H	-5.804478420	-1.542843109	-0.808015056
H	-5.687314407	0.775816054	-1.749924127
H	-3.696774264	2.174315157	-1.359336097
C	-1.425306101	1.549686112	-0.120602009
O	-1.640691121	2.784153201	-0.055576004

H	2.045856147	-1.565237113	-0.500099039
H	3.020246218	2.517104183	0.469822035
O	4.027192289	0.216468013	0.103856009
C	4.545723328	-1.056176076	-0.161887010
H	5.614425406	-0.975135068	-0.034775005
H	4.331735309	-1.368587100	-1.178537086
H	4.162226300	-1.796543129	0.532035039
H	-0.309626022	-0.977561070	-0.615850042
O	0.570385043	3.325343239	0.359566024
H	-0.473791034	3.302677239	0.188300014
C	2.604592189	6.073086437	1.860258133
O	2.831708201	5.271928380	0.740478053
H	2.038472145	4.793931345	0.531129040
H	1.869664132	6.851482494	1.663761121
H	3.540920255	6.550011470	2.118443152
H	2.267980165	5.493473394	2.716856196
C	-3.962119284	5.772214414	-0.844731061
O	-4.192426303	4.463730319	-0.412292028
H	-3.378357243	4.069506292	-0.122916011
H	-4.898123350	6.157496441	-1.226613088
H	-3.222918231	5.817632417	-1.641505117
H	-3.635063264	6.418937461	-0.033927003

1.2 angstrom

C	-2.651767193	-0.647523047	0.273840019
C	-3.830862275	-1.427471102	0.076859005
C	-4.927138356	-0.922714066	-0.665452048
C	-4.857360350	0.396468030	-1.180413083
C	-3.699604267	1.198745085	-0.966191067
C	-2.552537182	0.672113046	-0.279548021
C	-0.036853004	1.084562081	-0.058736002
C	0.405952029	-0.233302015	-0.329632023
C	0.963657070	2.095135149	0.199771016
C	1.760256127	-0.570749043	-0.285920019
C	2.307600169	1.747218126	0.269116022
C	2.705696197	0.424037032	0.026948002
H	-1.875259134	-1.027833073	0.905760063
H	-3.883556280	-2.406516171	0.513288035
H	-5.803997419	-1.521680110	-0.810752056
H	-5.677518410	0.809470060	-1.733751126
H	-3.682158266	2.204949159	-1.328855096
C	-1.391110101	1.540331110	-0.113884008
O	-1.610347118	2.779201203	-0.032178004
H	2.057897147	-1.575011112	-0.509975036
H	3.040424217	2.501847182	0.477514034
O	4.030184289	0.202406017	0.103429006
C	4.547076328	-1.070993076	-0.161679012

H	5.615629406	-0.990924071	-0.032091002
H	4.335703313	-1.383094097	-1.178843083
H	4.161915298	-1.811446131	0.530998037
H	-0.294659021	-0.986749069	-0.623959043
O	0.578482043	3.317348239	0.357399027
H	-0.533339038	3.265200234	0.177247015
C	2.584725187	6.059107436	1.854658131
O	2.812554202	5.258536380	0.735841052
H	2.028817148	4.756747340	0.542674036
H	1.833262130	6.823736493	1.665178121
H	3.514932255	6.554901470	2.100288150
H	2.269324164	5.477292392	2.718045193
C	-3.951723284	5.803675420	-0.866144060
O	-4.172949299	4.494588322	-0.427837033
H	-3.363066243	4.121479298	-0.102920006
H	-4.882793350	6.168804446	-1.278179093
H	-3.190614230	5.853305419	-1.641545118
H	-3.659017266	6.462051463	-0.051853004

1.1 angstrom

C	-2.630567188	-0.659274047	0.256284018
C	-3.801668275	-1.463082106	0.053284006
C	-4.918128356	-0.962551069	-0.664998046
C	-4.877117352	0.374097025	-1.143053084
C	-3.724309266	1.197175084	-0.931424069
C	-2.544236185	0.674823047	-0.283600021
C	-0.051631004	1.124988079	-0.057556006
C	0.401182031	-0.214194017	-0.328521026
C	0.955004070	2.131621153	0.193259013
C	1.715498125	-0.553004042	-0.284556022
C	2.321402170	1.739285124	0.272838022
C	2.696481194	0.460712032	0.041419005
H	-1.856801135	-1.029894076	0.897123065
H	-3.830070277	-2.450042174	0.473159032
H	-5.786836418	-1.572264116	-0.812358061
H	-5.713915412	0.787736058	-1.670189122
H	-3.739675267	2.213762157	-1.261367089
C	-1.391192102	1.538945110	-0.123947007
O	-1.663780119	2.815331203	-0.060838005
H	2.019176147	-1.551852114	-0.523680039
H	3.056354220	2.490119180	0.489887034
O	3.998507289	0.180621012	0.114194011
C	4.491382323	-1.108957078	-0.141128011
H	5.558424398	-1.045930078	0.004092001
H	4.289368310	-1.417201100	-1.160433086
H	4.082600296	-1.836960131	0.549703040
H	-0.305393022	-0.961164069	-0.625187047

O	0.626520044	3.343306240	0.340718027
H	-0.696398048	3.306942238	0.119415011
C	2.597508189	6.040041434	1.837371133
O	2.854308208	5.226474378	0.735319051
H	2.077279147	4.714155340	0.535738036
H	1.842226133	6.794481490	1.623160119
H	3.517547253	6.549212470	2.095006151
H	2.270333163	5.467907391	2.703061196
C	-4.070594291	5.781378415	-0.744223056
O	-4.264253309	4.478655324	-0.275763022
H	-3.432000247	4.100899293	-0.018603999
H	-5.030658364	6.152092441	-1.077694080
H	-3.379027244	5.817246419	-1.582972112
H	-3.702871264	6.444899464	0.034740005

1.0 angstrom

C	-2.614957189	-0.660074046	0.246321018
C	-3.783385270	-1.471100105	0.048551002
C	-4.906789353	-0.973206069	-0.653264049
C	-4.882613350	0.362075028	-1.125613080
C	-3.733571270	1.194027088	-0.922460066
C	-2.542511184	0.678889049	-0.286258020
C	-0.061194004	1.148612081	-0.062277002
C	0.387213027	-0.200440012	-0.341440026
C	0.979177072	2.161767158	0.199158017
C	1.692329120	-0.552388037	-0.296781022
C	2.347275169	1.728020126	0.281111020
C	2.695605194	0.453308033	0.043803001
H	-1.834696131	-1.027208072	0.880528066
H	-3.802713273	-2.460455176	0.462909033
H	-5.771706415	-1.589450115	-0.798089056
H	-5.726892409	0.769127058	-1.645823119
H	-3.759001269	2.208530160	-1.256820092
C	-1.398018102	1.541444113	-0.137688010
O	-1.724134123	2.837631203	-0.106740010
H	1.986997143	-1.552048111	-0.542955040
H	3.093025224	2.465593175	0.505997036
O	3.989714290	0.138212011	0.120321010
C	4.458834318	-1.157561082	-0.147365010
H	5.526120397	-1.115532079	0.004236000
H	4.257704307	-1.451149107	-1.171112084
H	4.034288292	-1.886127138	0.533207040
H	-0.324031026	-0.937563065	-0.649966047
O	0.688810049	3.354811242	0.349502025
H	-0.882235065	3.356972243	0.039860001
C	2.611255187	6.054658437	1.841676132
O	2.906569208	5.253955378	0.740241055

H	2.150399156	4.712675337	0.536601040
H	1.837193133	6.788058490	1.620533119
H	3.512281251	6.589441472	2.114607152
H	2.288801163	5.469505395	2.700455193
C	-4.124755296	5.787877415	-0.730590053
O	-4.348197315	4.488754323	-0.263772019
H	-3.525485256	4.098115297	0.002888001
H	-5.076558368	6.181663443	-1.060770076
H	-3.434733247	5.808311420	-1.571143112
H	-3.739281268	6.440796461	0.048730001

S₁ state minimum-energy proton transfer path

2.1 angstrom

3	C	-2.545250184	-0.782042057	0.261420017
4	C	-3.680641263	-1.576236115	0.124998011
5	C	-4.793766347	-1.102078080	-0.555625041
6	C	-4.771452345	0.194031014	-1.090514081
7	C	-3.669317262	0.986644070	-0.961577070
8	C	-2.504846178	0.510357039	-0.301424023
9	C	0.064005004	0.980752073	-0.116557009
10	C	0.518421039	-0.285990018	-0.513839036
11	C	1.054626074	1.885308135	0.352621028
12	C	1.859994132	-0.654852046	-0.456712034
13	C	2.384662172	1.529515108	0.391039026
14	C	2.796089201	0.250946017	-0.017485001
15	H	-1.705765121	-1.151708085	0.818526061
16	H	-3.696498266	-2.558752184	0.560308043
17	H	-5.667693409	-1.716907123	-0.662223046
18	H	-5.630975403	0.566026041	-1.616744114
19	H	-3.682103264	1.975556140	-1.378782102
20	C	-1.339641099	1.348153095	-0.208036013
21	O	-1.578431115	2.689718192	-0.442020031
22	H	2.138669153	-1.637289120	-0.783881054
23	H	3.114399223	2.227306163	0.753184053
24	O	4.118146296	0.023148001	0.071238005
25	C	4.629837332	-1.227782088	-0.292166019
26	H	5.694462412	-1.175303083	-0.123305009
27	H	4.444196318	-1.442855105	-1.339113096
28	H	4.210285305	-2.019571146	0.319160023
29	H	-0.183955014	-0.988200073	-0.915301065
30	O	0.761654054	3.150103224	0.768008054
31	H	-0.147436010	3.247820233	1.015736071
32	C	3.378310241	5.632120405	1.623142116
33	O	2.127133153	5.852770421	1.047896077
34	H	1.741305126	5.018526362	0.813450061
35	H	3.323218238	4.963406360	2.479633179
36	H	3.755633268	6.587486474	1.963152141

37	H	4.091381294	5.219862377	0.911312063
38	C	-4.420860321	5.961699431	-0.604660044
39	O	-4.138316299	4.610204333	-0.375253028
40	H	-3.201185228	4.484727321	-0.331363025
41	H	-5.496695395	6.068141439	-0.608186042
42	H	-4.037447289	6.301702454	-1.563657111
43	H	-4.017269290	6.600492476	0.176879014

2.0 angstrom

C	-2.543083182	-0.789418058	0.256100018
C	-3.681833267	-1.579048115	0.118541006
C	-4.795367347	-1.096959079	-0.556403037
C	-4.770098345	0.203405013	-1.083579076
C	-3.665903264	0.991396071	-0.953023068
C	-2.500175178	0.506415039	-0.298798023
C	0.072623005	0.973026069	-0.120649010
C	0.530395039	-0.294087023	-0.510014037
C	1.059359078	1.884377138	0.343665025
C	1.872595134	-0.659259050	-0.448649034
C	2.390354172	1.531897110	0.386591027
C	2.805013204	0.251899018	-0.011653002
H	-1.703502121	-1.164824082	0.809096059
H	-3.699858266	-2.563714184	0.548887038
H	-5.672033408	-1.707635123	-0.663731048
H	-5.629672405	0.580705042	-1.605806116
H	-3.676245266	1.983113141	-1.363794098
C	-1.331875095	1.337692097	-0.206705016
O	-1.562423112	2.684918195	-0.425762028
H	2.154594155	-1.642895117	-0.769186056
H	3.118488223	2.234658160	0.742376053
O	4.127704295	0.027564002	0.080441006
C	4.642680332	-1.224058088	-0.275452020
H	5.706898410	-1.168609086	-0.104837009
H	4.459612320	-1.445088106	-1.321628096
H	4.223743304	-2.013702147	0.339090024
H	-0.170336013	-1.000645073	-0.906780068
O	0.761229056	3.147155226	0.757094054
H	-0.170027010	3.277302237	0.882039063
C	3.379052243	5.651740408	1.631267119
O	2.128879152	5.850843422	1.045789073
H	1.753431127	5.008965362	0.822098060
H	3.326933237	4.989017359	2.492478179
H	3.741304270	6.614741473	1.966189142
H	4.102391297	5.243493379	0.927418065
C	-4.428774320	5.966577429	-0.606240046
O	-4.122689298	4.617248333	-0.393464028
H	-3.183857229	4.509251326	-0.342725027

H	-5.506267397	6.053577434	-0.612515046
H	-4.047943292	6.325780453	-1.559220113
H	-4.039583292	6.601884477	0.185301013

1.9 angstrom

C	-2.536483183	-0.795151058	0.250650016
C	-3.678359266	-1.580371116	0.114206007
C	-4.793393346	-1.091133081	-0.552660040
C	-4.766871342	0.213246017	-1.072006075
C	-3.660759264	0.997504073	-0.941299067
C	-2.492705180	0.504325037	-0.296250019
C	0.083964004	0.962658068	-0.125583011
C	0.545732041	-0.303065023	-0.512302035
C	1.064727078	1.880610137	0.336596022
C	1.889165134	-0.662475045	-0.445249034
C	2.397111172	1.533851113	0.385286028
C	2.816527201	0.253599021	-0.006687001
H	-1.695191123	-1.176293083	0.797011058
H	-3.697122267	-2.567530187	0.538797040
H	-5.672259409	-1.698612121	-0.660284045
H	-5.627635405	0.595590042	-1.588427115
H	-3.670414262	1.991955142	-1.345615097
C	-1.320325097	1.327970095	-0.209711018
O	-1.538972109	2.679693194	-0.421135030
H	2.176360157	-1.645812117	-0.761967057
H	3.122227225	2.240823159	0.739028054
O	4.139665299	0.033750004	0.090008007
C	4.659637335	-1.217258086	-0.260710020
H	5.723125414	-1.158100081	-0.086920004
H	4.480625324	-1.441789104	-1.306847096
H	4.241236305	-2.006464145	0.354749024
H	-0.151725013	-1.013086073	-0.908908064
O	0.753568056	3.139014225	0.751087056
H	-0.183536011	3.289794239	0.762324056
C	3.378158245	5.666608410	1.626182118
O	2.126092155	5.841075419	1.036966074
H	1.754690124	4.991048357	0.838749062
H	3.331842240	5.024748359	2.503248179
H	3.732730270	6.640385477	1.937221138
H	4.104390296	5.247125377	0.932022066
C	-4.440011319	5.969456428	-0.598164044
O	-4.096765297	4.624175332	-0.417763027
H	-3.155911225	4.542810329	-0.356940024
H	-5.519397396	6.025083435	-0.615552047
H	-4.058735291	6.364923456	-1.536421109
H	-4.078680294	6.593871474	0.214886017

1.8 angstrom

C	-2.495826177	-0.776370055	0.228548018
C	-3.652177264	-1.538666112	0.086709005
C	-4.767815342	-1.014886074	-0.552457042
C	-4.726632339	0.302938020	-1.037250073
C	-3.606934260	1.065987075	-0.900610067
C	-2.437589173	0.536499041	-0.285213022
C	0.148612011	0.958934068	-0.118355011
C	0.607082046	-0.306913020	-0.505087037
C	1.129616083	1.878461137	0.340640026
C	1.950560141	-0.667744047	-0.432747030
C	2.460885175	1.530713113	0.394138031
C	2.877905206	0.247290016	0.008066000
H	-1.655058119	-1.185088083	0.755300053
H	-3.681741264	-2.535684183	0.486593033
H	-5.657749406	-1.605259116	-0.664733050
H	-5.587918404	0.711939053	-1.532203112
H	-3.606053259	2.071844148	-1.276075089
C	-1.251848090	1.337390095	-0.197334017
O	-1.444516103	2.698269194	-0.373724029
H	2.236957160	-1.652268117	-0.746444055
H	3.186518229	2.237486162	0.747242054
O	4.200191302	0.023800001	0.111092006
C	4.716314341	-1.231949089	-0.227258017
H	5.778919418	-1.177173084	-0.047413001
H	4.542829327	-1.463055108	-1.272854093
H	4.290204310	-2.014444143	0.391395030
H	-0.090414008	-1.015875075	-0.903864063
O	0.808370060	3.134578228	0.753453055
H	-0.128248011	3.289614239	0.702268053
C	3.327915242	5.769763413	1.622514115
O	2.086792151	5.872027425	0.994360072
H	1.754728125	5.000665359	0.819357060
H	3.281404234	5.160402370	2.522139183
H	3.636005263	6.767626485	1.905553139
H	4.088923292	5.353864386	0.964436067
C	-4.415372319	5.992305429	-0.649637047
O	-3.861623280	4.706789341	-0.686154050
H	-2.916688209	4.766737344	-0.685888048
H	-5.490392397	5.879300421	-0.620688045
H	-4.150701296	6.572650472	-1.530013112
H	-4.107749296	6.541228472	0.236142019

4.7 angstrom

C	-2.491961178	-0.783117055	0.220939016
C	-3.652492262	-1.537292109	0.076862006
C	-4.766983343	-1.001190073	-0.555778042

C	-4.719078339	0.320235025	-1.030409076
C	-3.595225261	1.076557079	-0.890459067
C	-2.427614177	0.535005041	-0.281950020
C	0.161616013	0.941970069	-0.117466009
C	0.623614046	-0.323446025	-0.496567034
C	1.137842080	1.871424133	0.332095025
C	1.970089141	-0.675379048	-0.422084030
C	2.469787180	1.532527111	0.390393028
C	2.891657210	0.246982019	0.013881002
H	-1.651417120	-1.199777086	0.741744051
H	-3.687098263	-2.537973182	0.467970031
H	-5.660611409	-1.585680113	-0.670849048
H	-5.578444401	0.738112054	-1.520868109
H	-3.588638258	2.085719149	-1.257502090
C	-1.236884090	1.325006094	-0.192713014
O	-1.415746101	2.693854194	-0.342040023
H	2.263321162	-1.659777121	-0.729496053
H	3.193089229	2.245267163	0.735923054
O	4.214546304	0.030241003	0.120197008
C	4.736881338	-1.224731090	-0.210933015
H	5.799100418	-1.163689082	-0.030613004
H	4.565152330	-1.462543108	-1.255305089
H	4.313951308	-2.005918145	0.411530029
H	-0.069637006	-1.038921077	-0.891045062
O	0.796336056	3.126654227	0.729505054
H	-0.139293009	3.273672235	0.619463042
C	3.318630239	5.765547416	1.619676116
O	2.079224149	5.861796423	0.987359073
H	1.742360125	4.989023359	0.828431058
H	3.268214237	5.172573373	2.530206183
H	3.631150263	6.767335485	1.884121138
H	4.079002293	5.333356381	0.971123068
C	-4.419018318	5.981081431	-0.643203045
O	-3.786477274	4.739906343	-0.783924055
H	-2.847732207	4.858776349	-0.788384056
H	-5.483590395	5.797008416	-0.612809046
H	-4.207754303	6.640001479	-1.480659105
H	-4.130577299	6.483075469	0.276534018

1.6 angstrom

C	-2.463243178	-0.711932052	0.188224014
C	-3.649001264	-1.424253101	0.027186000
C	-4.747440340	-0.833663060	-0.588925043
C	-4.655256335	0.498199038	-1.030022073
C	-3.507322252	1.212725085	-0.873263060
C	-2.357513172	0.616298044	-0.279118022
C	0.244368016	0.956812067	-0.098601009

C	0.690453049	-0.315087025	-0.470212034
C	1.230757091	1.880315136	0.343490027
C	2.035007146	-0.678163050	-0.395904028
C	2.558418183	1.529708110	0.403327030
C	2.965736215	0.237513017	0.033634003
H	-1.637503119	-1.169084086	0.698168051
H	-3.715113266	-2.432901176	0.393232026
H	-5.660597407	-1.384241099	-0.717586051
H	-5.499427395	0.956720070	-1.510638107
H	-3.462833252	2.227805161	-1.223098086
C	-1.144726084	1.368801099	-0.169126012
O	-1.286733095	2.747943200	-0.269558017
H	2.318983168	-1.667016122	-0.697912051
H	3.289845236	2.237460159	0.742473051
O	4.287124307	0.008056999	0.139848011
C	4.795533344	-1.254672092	-0.181687013
H	5.858455420	-1.203229089	-0.002133002
H	4.621190333	-1.499330108	-1.224162087
H	4.364775317	-2.026686146	0.447023031
H	-0.009922999	-1.027056071	-0.858505064
O	0.889045063	3.139251228	0.725916053
H	-0.049072003	3.281132237	0.592942044
C	3.292486237	5.849651419	1.646813119
O	2.076049149	5.897646425	0.966223072
H	1.778894126	5.011610359	0.802277060
H	3.227465234	5.259218379	2.557748186
H	3.558471255	6.863226493	1.917431137
H	4.092400293	5.442356390	1.030648074
C	-4.232413307	5.901906423	-0.756829053
O	-3.428273247	4.922416354	-1.354246100
H	-2.515757183	5.114797367	-1.193197084
H	-5.261178377	5.632532406	-0.951700067
H	-4.048388293	6.887535494	-1.176633085
H	-4.088403296	5.947779428	0.319979025

1.5 angstrom

C	-2.468687179	-0.714477050	0.177250015
C	-3.659565266	-1.417108103	0.012166002
C	-4.754881340	-0.813136057	-0.598157043
C	-4.653227337	0.522869038	-1.028138075
C	-3.501271253	1.228010089	-0.866202063
C	-2.354278169	0.617367045	-0.278568022
C	0.252099020	0.937604066	-0.098511007
C	0.702552051	-0.333556025	-0.459805033
C	1.230810088	1.873374135	0.334563023
C	2.051074147	-0.685106051	-0.382187028
C	2.560013187	1.534613112	0.398669026

C	2.974405212	0.241096017	0.040166003
H	-1.645531119	-1.181285088	0.682597047
H	-3.731912268	-2.428349172	0.369951027
H	-5.672116410	-1.355785096	-0.730897055
H	-5.494258397	0.990865073	-1.504798107
H	-3.448680248	2.245436161	-1.208364088
C	-1.134509084	1.355571096	-0.167515011
O	-1.259028089	2.740730196	-0.249604018
H	2.342718170	-1.674184119	-0.675899050
H	3.287616235	2.250781164	0.728394052
O	4.297655310	0.020805000	0.146951009
C	4.813657348	-1.240907091	-0.165962013
H	5.876473424	-1.181899087	0.011396001
H	4.639289332	-1.494386105	-1.206315087
H	4.388772314	-2.011032146	0.469012034
H	0.007008000	-1.053891078	-0.841788058
O	0.862499061	3.129705225	0.697106050
H	-0.079568007	3.247986236	0.526006038
C	3.275288236	5.832300422	1.644307116
O	2.063035151	5.886431423	0.957238071
H	1.756313127	5.002272360	0.799931058
H	3.199681232	5.251532376	2.560735186
H	3.550779256	6.845516492	1.906407136
H	4.074152293	5.410767387	1.036333073
C	-4.219534302	5.892636423	-0.768025057
O	-3.392386245	4.931850356	-1.364156098
H	-2.484747179	5.142355373	-1.197162088
H	-5.241249377	5.611005402	-0.980820072
H	-4.043890292	6.884868493	-1.174328084
H	-4.091499295	5.928758427	0.310479024

1.4 angstrom

C	-2.479356181	-0.709131053	0.146709011
C	-3.683647265	-1.385545098	-0.027416001
C	-4.772147345	-0.747108056	-0.617059043
C	-4.647839334	0.596881044	-1.017632076
C	-3.482560249	1.276221089	-0.847469061
C	-2.343143168	0.631486045	-0.278868017
C	0.271261020	0.917404068	-0.095331006
C	0.720423050	-0.356806026	-0.441894034
C	1.249146090	1.862035132	0.322285021
C	2.071297148	-0.703082049	-0.363568027
C	2.577902188	1.527623109	0.390455026
C	2.992857215	0.229874015	0.046335003
H	-1.662835119	-1.201803089	0.637696046
H	-3.773227274	-2.402925174	0.308430023
H	-5.700046412	-1.269442091	-0.756284053

H	-5.482301393	1.091440078	-1.478719109
H	-3.412064246	2.299080166	-1.169687083
C	-1.111541082	1.345521094	-0.158691012
O	-1.218528090	2.738180197	-0.197927013
H	2.365088170	-1.694886121	-0.645671048
H	3.305602240	2.249023163	0.708389051
O	4.317072311	0.013409002	0.153051009
C	4.835713350	-1.249486092	-0.150005012
H	5.899035425	-1.185775088	0.022962001
H	4.658372337	-1.513236108	-1.187326085
H	4.415454320	-2.015011146	0.493580035
H	0.026330002	-1.083945076	-0.813263060
O	0.865111064	3.119619223	0.659209048
H	-0.087638007	3.213770233	0.476544036
C	3.244371235	5.822952421	1.640006117
O	2.042054146	5.878747425	0.935867068
H	1.735334122	4.994705358	0.776476055
H	3.152375226	5.251115379	2.560651184
H	3.523303251	6.836782490	1.896650134
H	4.048835289	5.390583387	1.047011076
C	-4.239669306	5.851675421	-0.775505057
O	-3.367282240	4.933071353	-1.374336097
H	-2.470865177	5.197399374	-1.222829089
H	-5.246493375	5.509261397	-0.969821070
H	-4.127440299	6.847629491	-1.195034086
H	-4.097826297	5.907379423	0.300411019

1.3 angstrom

C	-2.482255178	-0.709259050	0.134873009
C	-3.692816267	-1.372573101	-0.044779005
C	-4.776926345	-0.717056054	-0.626547043
C	-4.640432334	0.631845044	-1.012233071
C	-3.470124251	1.298387091	-0.836054063
C	-2.334632167	0.635412048	-0.276293020
C	0.284993022	0.898563067	-0.094605007
C	0.736518055	-0.375301025	-0.429632029
C	1.256730089	1.855975131	0.310365023
C	2.091487149	-0.710787050	-0.350543023
C	2.586013184	1.531665108	0.381757030
C	3.006541215	0.231982019	0.049748006
H	-1.669533122	-1.213668089	0.620047042
H	-3.791180273	-2.392641170	0.280180023
H	-5.709732408	-1.228963090	-0.770900056
H	-5.470951393	1.138700083	-1.466923108
H	-3.389486242	2.323742165	-1.148026081
C	-1.095771081	1.332240095	-0.152769011
O	-1.187537084	2.732095199	-0.167735011

H	2.392013174	-1.703169121	-0.623211046
H	3.311461237	2.259919161	0.688980052
O	4.332512311	0.023539000	0.156862012
C	4.857021349	-1.238879088	-0.136477009
H	5.920390426	-1.168565085	0.033785004
H	4.679116339	-1.512482110	-1.171170087
H	4.442012319	-2.001354145	0.514162035
H	0.046047004	-1.110341077	-0.792456059
O	0.847900060	3.110266221	0.624559046
H	-0.119757008	3.178164229	0.424609031
C	3.222916231	5.807147420	1.638879117
O	2.027249148	5.868182423	0.924322066
H	1.714803125	4.985787361	0.765843053
H	3.118969224	5.241053375	2.561822184
H	3.507382250	6.820194493	1.892464136
H	4.029223287	5.365608385	1.055241078
C	-4.244047306	5.845788419	-0.780292058
O	-3.337277239	4.946685354	-1.357608095
H	-2.452228174	5.253797376	-1.221398088
H	-5.237085376	5.459609394	-0.963221071
H	-4.171453299	6.834006490	-1.225679090
H	-4.102480294	5.934650430	0.293328019

1.2 angstrom

C	-2.488103179	-0.712171049	0.113010008
C	-3.707488267	-1.355881099	-0.072017007
C	-4.790105346	-0.672479046	-0.629160046
C	-4.639862336	0.686615048	-0.981842072
C	-3.462066252	1.333987094	-0.800206056
C	-2.326993165	0.642230047	-0.266704021
C	0.298942023	0.874210065	-0.088732007
C	0.753804053	-0.397277031	-0.417000028
C	1.264147090	1.843446135	0.306379022
C	2.114090151	-0.720916053	-0.338859022
C	2.595218185	1.529622108	0.378255030
C	3.021793220	0.230231019	0.053468006
H	-1.677749123	-1.237031090	0.579585044
H	-3.815627273	-2.382332173	0.228714016
H	-5.730151411	-1.169262085	-0.778451055
H	-5.468792392	1.214648089	-1.414766102
H	-3.371245243	2.365470172	-1.088340078
C	-1.079171077	1.315211097	-0.141617008
O	-1.153729082	2.723363197	-0.138924009
H	2.421813172	-1.712495123	-0.606273045
H	3.317179241	2.265264163	0.675910046
O	4.350820315	0.030878000	0.157771011
C	4.881756353	-1.228732088	-0.133349010

H	5.945617427	-1.151444084	0.031156004
H	4.700704337	-1.507821106	-1.166157085
H	4.475158320	-1.991875141	0.522003040
H	0.068945006	-1.140834080	-0.773063057
O	0.832374058	3.093261222	0.602384042
H	-0.159361009	3.138595228	0.389105026
C	3.205120233	5.784649418	1.632146120
O	2.012079144	5.847764420	0.913520066
H	1.694001119	4.966181360	0.760401052
H	3.093909220	5.230272378	2.561448183
H	3.497686252	6.798134490	1.874815133
H	4.009359291	5.329544384	1.056066076
C	-4.240729306	5.851680422	-0.788754057
O	-3.294916235	4.970318357	-1.330070098
H	-2.424694177	5.323946382	-1.211061087
H	-5.215788373	5.414999387	-0.953983070
H	-4.211762302	6.822752493	-1.274706092
H	-4.103020293	5.991076430	0.279931018

1.1 angstrom

C	-2.508816182	-0.654271046	0.264712018
C	-3.627069258	-1.431067105	0.142273008
C	-4.738689341	-0.980821072	-0.578834041
C	-4.707055337	0.284597023	-1.153023085
C	-3.578650260	1.091580077	-1.024629074
C	-2.439786174	0.627570043	-0.335824026
C	0.120275009	1.014889075	-0.121263009
C	0.555519042	-0.260034017	-0.519864036
C	1.139670081	1.885518134	0.335411025
C	1.878187135	-0.662137049	-0.446983031
C	2.465728179	1.507981108	0.399420029
C	2.840384205	0.220417014	0.008959003
H	-1.681160120	-1.012285073	0.847834061
H	-3.658268263	-2.397011174	0.613617047
H	-5.609107402	-1.603185117	-0.673950048
H	-5.552436397	0.644634046	-1.709963121
H	-3.575109260	2.069853150	-1.463616105
C	-1.260693092	1.457768103	-0.245723016
O	-1.451096104	2.805979201	-0.410037029
H	2.137481156	-1.650202119	-0.773089056
H	3.215957232	2.190745158	0.749331056
O	4.155359299	-0.046801002	0.105267008
C	4.634974331	-1.310881093	-0.257544021
H	5.698746408	-1.288174092	-0.077572003
H	4.454414323	-1.517749111	-1.306999097
H	4.187918300	-2.092329149	0.347213027
H	-0.161957010	-0.944196069	-0.927360067

O	0.847887059	3.152257225	0.751457052
H	-0.966086068	3.150333226	-1.335341095
C	3.271171237	5.654298409	1.531211111
O	2.020888146	6.215055448	1.264668092
H	1.407214102	5.527184398	1.047312077
H	3.229338230	4.922086353	2.334705167
H	3.925314281	6.457816463	1.839771131
H	3.703972265	5.181119373	0.651903047
C	-4.583702332	5.295345384	-0.206274017
O	-3.574127255	4.783457345	-1.027028073
H	-3.004258217	4.220751304	-0.518641039
H	-5.236789376	5.893365423	-0.826697061
H	-4.186326302	5.931663425	0.580634043
H	-5.175444371	4.506646324	0.253104018

1.0 angstrom

C	-2.554791186	-0.704498053	0.285262019
C	-3.654166261	-1.509880108	0.172769011
C	-4.772250344	-1.099545078	-0.560186041
C	-4.767576344	0.153159009	-1.161296084
C	-3.656921264	0.986390070	-1.047741076
C	-2.513334181	0.564626039	-0.341890022
C	0.035938004	1.009016075	-0.139583009
C	0.486790035	-0.263986019	-0.528655036
C	1.046983077	1.891450137	0.314805021
C	1.814767131	-0.651502047	-0.452642031
C	2.377313170	1.529225109	0.380051026
C	2.767111201	0.243377020	-0.003490998
H	-1.722212125	-1.030485077	0.880246062
H	-3.666375264	-2.466527178	0.663064046
H	-5.628038406	-1.743157124	-0.643130045
H	-5.620249403	0.484919034	-1.724405125
H	-3.674079264	1.952182143	-1.511354110
C	-1.352998099	1.424310104	-0.262306018
O	-1.584009115	2.768228199	-0.428085032
H	2.083813147	-1.639367119	-0.771384057
H	3.119351226	2.221703160	0.728262054
O	4.085283293	-0.008306003	0.093488009
C	4.580840329	-1.264775091	-0.275669019
H	5.645608408	-1.227557087	-0.103402007
H	4.395554319	-1.471545106	-1.324314094
H	4.149379300	-2.054095146	0.330202026
H	-0.223011015	-0.959563069	-0.929646065
O	0.739413052	3.156772228	0.725027051
H	-1.089107078	3.116462226	-1.224217090
C	3.275316235	5.631075407	1.538681109
O	2.032582149	6.192720448	1.237777087

H	1.413122101	5.502459395	1.046348075
H	3.216613232	4.924405356	2.363496172
H	3.931574284	6.438815465	1.831141134
H	3.715873265	5.128010367	0.680071051
C	-4.329429314	5.715090413	-0.256749017
O	-4.202219305	4.388143318	-0.673853049
H	-3.426061249	3.996987286	-0.294018023
H	-5.264261380	6.091465440	-0.649015046
H	-3.523697256	6.342908455	-0.632103044
H	-4.356425312	5.801302420	0.826415062

T₁ state minimum-energy proton transfer path
1.9 angstrom

C	-2.578486188	-0.735807053	0.390876029
C	-3.664826262	-1.583054114	0.168210011
C	-4.704628340	-1.179017087	-0.660382049
C	-4.668483337	0.078489004	-1.256158091
C	-3.611395261	0.926666067	-1.023365076
C	-2.547440184	0.524556039	-0.206564016
C	-0.033370002	1.089458076	-0.026326002
C	0.351649024	-0.275816019	-0.541001037
C	1.005283074	1.986073141	0.199334016
C	1.743178127	-0.749114056	-0.360360028
C	2.353191170	1.565669112	0.104642007
C	2.690949196	0.139226010	-0.102580010
H	-1.777685130	-1.052686078	1.033468075
H	-3.698261268	-2.548139185	0.638848048
H	-5.537050399	-1.835154134	-0.834141060
H	-5.472475392	0.393670026	-1.895383136
H	-3.605607258	1.906053138	-1.462526105
C	-1.440857101	1.499104107	0.050867004
O	-1.738941127	2.665981190	0.277831021
H	1.945814140	-1.792959128	-0.502702035
H	3.148413228	2.270417164	0.237104015
O	4.006073291	-0.072519006	0.031629004
C	4.503075325	-1.369144101	-0.158121009
H	5.571480402	-1.306192096	-0.020529003
H	4.285357311	-1.725813123	-1.158858085
H	4.085593296	-2.056856149	0.568679039
H	-0.150002012	-0.594185044	-1.437738104
O	0.831180060	3.276348236	0.555861038
H	-0.098118008	3.486479251	0.556524039
C	3.471170249	5.543593401	1.720880122
O	2.359988171	5.859396424	0.940463068
H	1.917111138	5.057327363	0.695296052
H	3.209706231	4.916922356	2.570750182
H	3.883127281	6.470683466	2.096949152

H	4.246486305	5.037338364	1.147316083
C	-4.298659308	5.563532403	-0.249057018
O	-4.477743324	4.178010303	-0.207614015
H	-3.695704267	3.764223270	0.133435012
H	-5.220090378	5.998552430	-0.611517044
H	-3.494331252	5.853720421	-0.921711068
H	-4.091298292	5.978250428	0.734430054

4.8 angstrom

C	-2.579617188	-0.732651050	0.391769026
C	-3.668819264	-1.576774113	0.169698010
C	-4.707523341	-1.169092082	-0.658489049
C	-4.667750337	0.088577006	-1.253891090
C	-3.607982258	0.933574069	-1.021513072
C	-2.544964185	0.527299040	-0.205827015
C	-0.028688000	1.077633076	-0.026056000
C	0.358513025	-0.286562022	-0.538686040
C	1.005040070	1.979105141	0.199787013
C	1.753076129	-0.752222052	-0.357582027
C	2.355718171	1.566062111	0.105266007
C	2.697510195	0.140301013	-0.100651005
H	-1.779571128	-1.051781074	1.034206076
H	-3.704725268	-2.541888183	0.640175045
H	-5.542101396	-1.822458129	-0.832415059
H	-5.471094393	0.406445027	-1.892575136
H	-3.599364258	1.913075140	-1.460393103
C	-1.432765103	1.494511107	0.050909005
O	-1.719776126	2.664746191	0.278406019
H	1.960942143	-1.795229129	-0.498078037
H	3.148060225	2.273476163	0.240693017
O	4.013003290	-0.067787002	0.035277003
C	4.514065326	-1.363130097	-0.152108010
H	5.582073403	-1.296922091	-0.012837999
H	4.299051312	-1.721511124	-1.152731085
H	4.097431293	-2.051168150	0.574755042
H	-0.141814010	-0.607563042	-1.435470103
O	0.812866061	3.266187234	0.553462040
H	-0.123918008	3.452284246	0.548630038
C	3.448436249	5.543425398	1.722648124
O	2.345712170	5.853067422	0.928179064
H	1.896374137	5.050601361	0.695875052
H	3.175644229	4.936080356	2.582970187
H	3.865883278	6.474306468	2.083166149
H	4.223604305	5.019216361	1.165074081
C	-4.294251309	5.569107402	-0.247717020
O	-4.463795323	4.182187300	-0.207989017
H	-3.679846264	3.773383270	0.134607007

H	-5.217800374	5.997971430	-0.612159042
H	-3.490202251	5.865464420	-0.917972066
H	-4.092349297	5.984260432	0.736721053

1.7 angstrom

C	-2.578294186	-0.733719052	0.386064030
C	-3.672532262	-1.570560112	0.161798013
C	-4.710339337	-1.152146085	-0.662147045
C	-4.664784336	0.108884008	-1.250352090
C	-3.600542259	0.947370069	-1.014782075
C	-2.538609184	0.529935036	-0.203613017
C	-0.017713002	1.057059077	-0.025661001
C	0.375162026	-0.308255024	-0.528353040
C	1.006741073	1.969721141	0.195789015
C	1.776527126	-0.755955053	-0.352568025
C	2.361440170	1.570898113	0.103201010
C	2.713142197	0.146258009	-0.099736005
H	-1.777978130	-1.061092075	1.023944075
H	-3.712341267	-2.538286185	0.626685047
H	-5.548928397	-1.799692130	-0.838549059
H	-5.467219392	0.434063031	-1.886414137
H	-3.587319257	1.929223137	-1.448123102
C	-1.416395100	1.484012109	0.051668004
O	-1.685342123	2.659671191	0.282153023
H	1.995547144	-1.796929132	-0.490791033
H	3.148134225	2.284324165	0.239735016
O	4.030428288	-0.051319001	0.034749001
C	4.541214325	-1.343620099	-0.147162013
H	5.608717404	-1.268634090	-0.008578000
H	4.328773314	-1.708014125	-1.146171081
H	4.129997300	-2.031737148	0.582763044
H	-0.127714008	-0.640924048	-1.419722101
O	0.779692055	3.251957235	0.537536038
H	-0.170943011	3.392983247	0.524742040
C	3.414315244	5.522148398	1.726384126
O	2.328440169	5.838056420	0.911876066
H	1.862965134	5.041230362	0.691705050
H	3.117451226	4.944453358	2.598976185
H	3.851272277	6.451420462	2.067302150
H	4.182232301	4.964738357	1.191591084
C	-4.285697307	5.578925402	-0.248687018
O	-4.435634320	4.189675301	-0.205905016
H	-3.647739260	3.792179275	0.140873011
H	-5.214102378	5.993272431	-0.617461043
H	-3.483646248	5.884874425	-0.916931069
H	-4.093237293	5.999344433	0.735348055

1.6 angstrom

C	-2.578087188	-0.732773052	0.382271030
C	-3.677273267	-1.562581114	0.156877014
C	-4.713461340	-1.134987079	-0.664481045
C	-4.661408333	0.128082008	-1.248088090
C	-3.592587259	0.960250069	-1.010647073
C	-2.532396183	0.533026040	-0.202798015
C	-0.007515000	1.037188075	-0.026937001
C	0.391022029	-0.327977026	-0.521462035
C	1.007168072	1.961019144	0.191904013
C	1.798335129	-0.759303057	-0.349237024
C	2.365953168	1.575154111	0.102318009
C	2.727184196	0.151750011	-0.098641005
H	-1.778190129	-1.066716075	1.017241072
H	-3.721769268	-2.531791180	0.618332042
H	-5.555947398	-1.776965126	-0.842685061
H	-5.462382394	0.459768033	-1.882522134
H	-3.574331258	1.943609138	-1.440355103
C	-1.400413100	1.473647104	0.051208006
O	-1.651587118	2.654750191	0.284257021
H	2.027943148	-1.798154130	-0.486007033
H	3.147462228	2.294421163	0.237652016
O	4.046024289	-0.035854002	0.034975002
C	4.566453328	-1.324763095	-0.143404013
H	5.633409407	-1.241375090	-0.005394999
H	4.356576313	-1.693586123	-1.141316081
H	4.160594302	-2.013947145	0.588519043
H	-0.113767007	-0.671943048	-1.407557099
O	0.746180054	3.236218233	0.523430040
H	-0.218448014	3.331930242	0.502307036
C	3.386043246	5.493954395	1.729233127
O	2.312407167	5.816944418	0.901795065
H	1.829331131	5.026791364	0.694938048
H	3.071638219	4.941048356	2.611767187
H	3.841865278	6.420067461	2.053787149
H	4.144785301	4.908847355	1.211079090
C	-4.276267310	5.591024405	-0.253691018
O	-4.407931319	4.199737305	-0.208300014
H	-3.617144259	3.813478273	0.144322008
H	-5.208556372	5.991919431	-0.627387043
H	-3.475463252	5.905914428	-0.919148067
H	-4.093760295	6.015989434	0.730217052

1.5 angstrom

C	-2.574454185	-0.734170053	0.373867028
C	-3.680352264	-1.554425111	0.146905013
C	-4.715787338	-1.113876082	-0.668580047

C	-4.656388335	0.152659011	-1.244242088
C	-3.581532260	0.976218071	-1.004012074
C	-2.522328183	0.535630036	-0.202275014
C	0.007300000	1.015407070	-0.026336003
C	0.4111113032	-0.351405026	-0.506927039
C	1.011559073	1.950813140	0.187271013
C	1.825411129	-0.764490052	-0.343560026
C	2.375482169	1.578169114	0.099095007
C	2.746628200	0.156000014	-0.098873007
H	-1.774486127	-1.078415078	1.003084072
H	-3.729780266	-2.526364181	0.602188046
H	-5.563504399	-1.748434127	-0.848646063
H	-5.456342392	0.493402036	-1.875057136
H	-3.557769254	1.962140142	-1.427252102
C	-1.379860099	1.461250105	0.051163005
O	-1.613357115	2.647847191	0.286412021
H	2.065294150	-1.801337131	-0.477630035
H	3.151280226	2.304632167	0.228415015
O	4.067367294	-0.020423003	0.030787003
C	4.597166331	-1.306184095	-0.142225011
H	5.663706408	-1.213907087	-0.007066998
H	4.388025317	-1.681669120	-1.137826083
H	4.198156303	-1.994726142	0.594096042
H	-0.100744008	-0.714490052	-1.381396100
O	0.718571051	3.219180234	0.505437035
H	-0.262303018	3.270466236	0.478768036
C	3.354346243	5.461951395	1.737430125
O	2.298972166	5.788519418	0.888542064
H	1.802064130	5.004085358	0.691026047
H	3.016725215	4.937904356	2.629045190
H	3.827345273	6.385310459	2.045379147
H	4.106449293	4.847495349	1.243823091
C	-4.263426306	5.606298402	-0.261878020
O	-4.373020316	4.212995301	-0.214594017
H	-3.579434257	3.839658275	0.145586012
H	-5.199523375	5.990989434	-0.642921046
H	-3.463105249	5.932580426	-0.922318066
H	-4.094811294	6.035894436	0.722443052

1.4 angstrom

C	-2.549956184	-0.746106054	0.352671024
C	-3.659465262	-1.560795114	0.122721009
C	-4.716575342	-1.093814078	-0.648721046
C	-4.675004336	0.193694013	-1.178132086
C	-3.596291257	1.010744072	-0.935530067
C	-2.515014181	0.544168041	-0.177983010
C	0.018766001	1.027568072	-0.013970999

C	0.449154034	-0.331520021	-0.486778033
C	0.999483074	1.987562145	0.190569015
C	1.875676136	-0.707389049	-0.331021023
C	2.376305172	1.652975119	0.083501005
C	2.777505200	0.235775019	-0.098777008
H	-1.734676122	-1.110144081	0.949954068
H	-3.697096268	-2.548128183	0.544554039
H	-5.567312401	-1.723834122	-0.830099062
H	-5.490966396	0.554936042	-1.775981127
H	-3.585592256	2.010756143	-1.324417093
C	-1.368268101	1.461737107	0.075894003
O	-1.599654113	2.648899190	0.326159022
H	2.137260155	-1.741192125	-0.448291030
H	3.129560225	2.408786172	0.177168014
O	4.101004297	0.085718004	0.032824002
C	4.653677334	-1.193036088	-0.117705007
H	5.718240409	-1.080267077	0.018270003
H	4.453876319	-1.588637114	-1.107479080
H	4.264624305	-1.876490137	0.628765047
H	-0.065448007	-0.722501049	-1.347300098
O	0.663988048	3.241798233	0.503200038
H	-0.338612023	3.237010232	0.480751032
C	3.017526215	5.560778400	2.041643145
O	2.704450196	5.393230390	0.692816047
H	1.982106143	4.780698342	0.612048047
H	2.153671154	5.864084421	2.634299189
H	3.764021272	6.342571459	2.109709150
H	3.432238245	4.653886332	2.485284178
C	-4.162753297	5.685669407	-0.314958022
O	-4.303356312	4.296725308	-0.221086016
H	-3.526856253	3.920623283	0.171680012
H	-5.072437363	6.073677438	-0.752564054
H	-3.327030240	5.970555429	-0.950079070
H	-4.030140288	6.148410442	0.659927046

1.3 angstrom

C	-2.554610186	-0.743177052	0.336204023
C	-3.670404266	-1.549674110	0.108596009
C	-4.731739339	-1.069305075	-0.648701048
C	-4.688493339	0.223591014	-1.165648085
C	-3.603546261	1.032561076	-0.925198066
C	-2.517787181	0.551861040	-0.182920012
C	0.019070003	1.022143073	-0.015846001
C	0.461208035	-0.336815022	-0.464028031
C	0.982774069	1.997985143	0.182947016
C	1.896627136	-0.688591049	-0.321813021
C	2.370574172	1.679702120	0.077698005

C	2.787680199	0.266721018	-0.100460009
H	-1.735288126	-1.117430079	0.921228067
H	-3.707384268	-2.541991182	0.518865040
H	-5.587475403	-1.692770121	-0.829173060
H	-5.508857397	0.595904045	-1.750775128
H	-3.591651261	2.036784144	-1.303067093
C	-1.363538098	1.457810104	0.068340003
O	-1.586743114	2.652176189	0.311696020
H	2.172196157	-1.719104124	-0.433754034
H	3.113031225	2.447037178	0.162449012
O	4.113856298	0.133008008	0.023260002
C	4.681386335	-1.138672084	-0.128909007
H	5.746005413	-1.012492071	-0.006641000
H	4.474287321	-1.540563112	-1.114531082
H	4.310365312	-1.824151131	0.624800044
H	-0.066689007	-0.766237057	-1.297071091
O	0.621780045	3.241854235	0.478400035
H	-0.413173029	3.194370230	0.448666032
C	3.032087220	5.447561394	2.053407147
O	2.804952200	5.213436376	0.697174050
H	2.015113145	4.696157339	0.596161045
H	2.198450159	5.947191428	2.532573182
H	3.893800278	6.090278437	2.135885152
H	3.237456233	4.530419326	2.594312186
C	-4.152366299	5.708981411	-0.322095025
O	-4.293600310	4.322232313	-0.206878014
H	-3.514309254	3.949921282	0.184138014
H	-5.066763366	6.090761438	-0.755243056
H	-3.323417240	5.984527433	-0.970379071
H	-4.008272287	6.187577443	0.643742044

1.2 angstrom

C	-2.553248185	-0.758430052	0.328324024
C	-3.676752266	-1.552591110	0.096261009
C	-4.734524341	-1.056169075	-0.655610045
C	-4.680301337	0.240643015	-1.161607081
C	-3.588574259	1.038641074	-0.915063068
C	-2.505783182	0.541259038	-0.179517010
C	0.029527000	0.991596073	-0.002588000
C	0.473319034	-0.364199024	-0.443909030
C	0.985560071	1.977554144	0.192467015
C	1.912811139	-0.711213053	-0.316158022
C	2.380857170	1.660424119	0.058994003
C	2.802867200	0.247229018	-0.110797010
H	-1.737134124	-1.143696082	0.910370064
H	-3.722372266	-2.547811185	0.498398035
H	-5.595734405	-1.670529119	-0.841031059

H	-5.497369398	0.624117045	-1.743777124
H	-3.568681259	2.045393149	-1.285073092
C	-1.342219097	1.429455104	0.076070007
O	-1.560992111	2.631205191	0.325353021
H	2.188502156	-1.742542125	-0.420450031
H	3.119170227	2.434115177	0.119420007
O	4.130805295	0.119864007	0.004224999
C	4.700463339	-1.151967080	-0.139366009
H	5.765477416	-1.021522073	-0.024547003
H	4.488804325	-1.563935114	-1.120004081
H	4.335681310	-1.831273132	0.623074047
H	-0.069893006	-0.817167060	-1.254230092
O	0.621156044	3.205118232	0.489650037
H	-0.476598033	3.129117224	0.452520035
C	3.004686216	5.439647389	2.046201149
O	2.675589192	5.300230383	0.697823048
H	1.946335142	4.695493338	0.611550043
H	2.152816157	5.737241413	2.653931189
H	3.757525272	6.211666448	2.125898154
H	3.417023245	4.523581324	2.466925178
C	-4.166937301	5.709715411	-0.336921027
O	-4.273187308	4.319690309	-0.219586015
H	-3.490487250	3.968784287	0.183885014
H	-5.085234366	6.066018438	-0.782843057
H	-3.337232238	6.004488433	-0.975211068
H	-4.048398290	6.192295444	0.630145046

1.1 angstrom

C	-2.603848187	-0.772234053	0.346748023
C	-3.710376267	-1.587976113	0.110351009
C	-4.757616345	-1.132252079	-0.680236049
C	-4.698368337	0.151416010	-1.223305090
C	-3.615164263	0.961893069	-0.986405072
C	-2.532665185	0.512787037	-0.210368018
C	-0.014260999	1.032781076	-0.031181002
C	0.443357034	-0.223953014	-0.405450031
C	1.053582076	2.039582148	0.263717017
C	1.849092134	-0.614543043	-0.415385032
C	2.445458176	1.619544118	0.225201015
C	2.829135204	0.294952021	-0.099274006
H	-1.819509130	-1.123270079	0.992146074
H	-3.758192269	-2.565741186	0.554560040
H	-5.610998406	-1.758661129	-0.861067059
H	-5.505590394	0.513148036	-1.833432133
H	-3.594406258	1.951447142	-1.398576098
C	-1.397168101	1.412708100	0.028592002
O	-1.756516125	2.716081194	0.155997013

H	2.080500149	-1.626867116	-0.679131047
H	3.184954230	2.364608169	0.444901031
O	4.156671299	0.064340005	-0.059652003
C	4.630736336	-1.233130091	-0.294879021
H	5.701412409	-1.186667085	-0.171168012
H	4.402394316	-1.563204114	-1.302625092
H	4.220282305	-1.939390140	0.419063031
H	-0.259101019	-0.968537069	-0.716956050
O	0.799656055	3.199503228	0.520264036
H	-0.845375059	3.295464235	0.369414028
C	3.170761230	5.576983401	2.067023147
O	2.745307199	5.520003399	0.738773054
H	2.085567148	4.845711349	0.647569048
H	2.344443166	5.704520409	2.759805200
H	3.829987275	6.426811460	2.166854155
H	3.725113266	4.687708336	2.358732169
C	-4.105835294	5.626901405	-0.287095020
O	-4.390559314	4.262184305	-0.224507015
H	-3.616580262	3.783989273	0.048628002
H	-4.999952362	6.130889441	-0.631057046
H	-3.299884236	5.848443423	-0.984348070
H	-3.839781277	6.036082437	0.686076049

1.0 angstrom

C	-2.629430187	-0.753108053	0.362235025
C	-3.721717266	-1.586884113	0.124012011
C	-4.769130342	-1.152817082	-0.677911050
C	-4.725631342	0.127052007	-1.229534088
C	-3.655653265	0.955503068	-0.991506071
C	-2.572140183	0.527437039	-0.206397013
C	-0.058310004	1.078043077	-0.038358000
C	0.402301029	-0.177954011	-0.401820028
C	1.000033074	2.096288152	0.249730021
C	1.809536129	-0.560438040	-0.416798030
C	2.395212172	1.678805123	0.224609019
C	2.783788201	0.355940027	-0.104872009
H	-1.844347133	-1.086969080	1.015499073
H	-3.758436272	-2.561905186	0.574950044
H	-5.611339403	-1.793480129	-0.860647062
H	-5.534212401	0.471793035	-1.847676135
H	-3.646382265	1.942277141	-1.411198103
C	-1.447638105	1.442007104	0.026718001
O	-1.826141129	2.743740199	0.124190010
H	2.046135145	-1.571352116	-0.681997050
H	3.131637225	2.425282172	0.451930034
O	4.113045297	0.131655008	-0.072377006
C	4.598362330	-1.142672082	-0.390517030

H	5.671735408	-1.086521079	-0.295744020
H	4.344014312	-1.420883105	-1.408082101
H	4.219142303	-1.893498138	0.295021021
H	-0.297503021	-0.927450065	-0.707372052
O	0.733810054	3.257101234	0.485659035
H	-1.016753075	3.310528239	0.277957018
C	3.083286220	5.740632412	1.997304145
O	3.127315228	5.003435359	0.810719056
H	2.261786162	4.661141336	0.624291044
H	2.488987180	6.646277479	1.892121134
H	4.097534297	6.025653433	2.243653162
H	2.680591192	5.158946370	2.824298201
C	-4.185405301	5.583093403	-0.235393016
O	-4.519306324	4.239955305	-0.058301003
H	-3.739340271	3.742912270	0.155861009
H	-5.091385364	6.112646442	-0.499787036
H	-3.461336252	5.725924412	-1.035463073
H	-3.786071273	6.030374435	0.672866049

S₀ state minimum-energy proton transfer path

1.9 angstrom

C	-2.637431189	-0.695595048	0.436158033
C	-3.736978267	-1.523800110	0.243698019
C	-4.750410342	-1.147863083	-0.635095044
C	-4.675607339	0.053070006	-1.303631095
C	-3.587005259	0.897287067	-1.110708078
C	-2.550899183	0.522000039	-0.253248017
C	-0.005549000	1.052874074	-0.040131003
C	0.369371027	-0.227380018	-0.454634034
C	1.038664077	1.944421139	0.317609020
C	1.693231124	-0.646326048	-0.487964036
C	2.357777168	1.530150110	0.286557021
C	2.689447195	0.231993015	-0.111990009
H	-1.867100136	-0.984384070	1.127377082
H	-3.807979275	-2.453741176	0.776626055
H	-5.595569402	-1.795063131	-0.779434055
H	-5.461169393	0.349656026	-1.973727140
H	-3.548627256	1.843053131	-1.616089115
C	-1.427195105	1.488841106	-0.036476003
O	-1.709663126	2.665927193	0.120122008
H	1.916141140	-1.642602117	-0.814793060
H	3.137568227	2.211928161	0.564997040
O	4.000131287	-0.051352006	-0.099748006
C	4.445979322	-1.319964093	-0.493115037
H	5.520039399	-1.300779094	-0.392400028
H	4.186598299	-1.527752112	-1.525463108
H	4.041023289	-2.096791151	0.146030013

H	-0.383459028	-0.916571064	-0.778715057
O	0.819464060	3.219030233	0.705953052
H	-0.100960008	3.438381246	0.605170044
C	3.567884255	5.470021396	1.689361124
O	2.387378174	5.792071415	1.022001074
H	1.924343139	4.991646359	0.810230059
H	3.390906242	4.822152346	2.545209183
H	4.005295289	6.392334462	2.047926146
H	4.290869311	4.984147356	1.035644073
C	-4.311069308	5.532672400	-0.254039016
O	-4.462977321	4.143584296	-0.278974022
H	-3.659670265	3.729799269	0.007872999
H	-5.254252378	5.967519428	-0.556090040
H	-3.540258255	5.873784420	-0.941803066
H	-4.071159293	5.899610424	0.741088051

1.8 angstrom

C	-2.638423189	-0.693906052	0.435445030
C	-3.740188267	-1.519150108	0.242605019
C	-4.752729340	-1.139797083	-0.635713044
C	-4.675302337	0.061698003	-1.303092096
C	-3.584865256	0.903284064	-1.109489081
C	-2.549363182	0.524066037	-0.253012020
C	-0.002705001	1.043923078	-0.041251002
C	0.374123029	-0.235928020	-0.454355031
C	1.037185074	1.939771137	0.315886025
C	1.699562121	-0.649491047	-0.485710037
C	2.357929169	1.531090109	0.287264023
C	2.692766195	0.233000018	-0.109752007
H	-1.868539133	-0.984954073	1.126236080
H	-3.813271275	-2.449401177	0.774775057
H	-5.599384405	-1.784879131	-0.780834057
H	-5.460222393	0.360617028	-1.972902142
H	-3.544456255	1.849762135	-1.613408118
C	-1.421440101	1.484743109	-0.035797005
O	-1.695457124	2.664026192	0.123917008
H	1.926835140	-1.645206119	-0.811217060
H	3.135710228	2.215490159	0.564962040
O	4.004064291	-0.047031004	-0.096307005
C	4.453813320	-1.314589097	-0.488812037
H	5.527768398	-1.292176090	-0.387627029
H	4.195525303	-1.523616110	-1.521173110
H	4.050864293	-2.092227150	0.150587012
H	-0.376768026	-0.927414065	-0.778435058
O	0.801576059	3.212128233	0.698759052
H	-0.125036011	3.409782243	0.590431045
C	3.551017254	5.468734395	1.686983123

O	2.373652173	5.787218415	1.012581073
H	1.905919139	4.986650359	0.811114061
H	3.368913244	4.834756348	2.552201181
H	3.992883289	6.394025458	2.032539148
H	4.272785308	4.969270358	1.042073074
C	-4.306445310	5.539796401	-0.252032016
O	-4.452288322	4.149927300	-0.278954019
H	-3.648453263	3.739527272	0.011243000
H	-5.250635378	5.970907432	-0.556276040
H	-3.535080255	5.884958421	-0.937198065
H	-4.070935292	5.906533427	0.744228051

1.7 angstrom

C	-2.641232189	-0.691243052	0.432645032
C	-3.747943269	-1.508648109	0.234867019
C	-4.754765344	-1.119984079	-0.645929049
C	-4.667592335	0.082887006	-1.309827094
C	-3.573244259	0.917833067	-1.109879079
C	-2.543501184	0.528725041	-0.251057017
C	0.006625003	1.026316075	-0.042243003
C	0.388417027	-0.254339017	-0.447361033
C	1.038645074	1.934319140	0.304471020
C	1.716876124	-0.656015045	-0.480088037
C	2.363237171	1.537465113	0.274889017
C	2.704541193	0.238315016	-0.113526009
H	-1.874455133	-0.988979070	1.124047080
H	-3.828740274	-2.439980176	0.764067055
H	-5.605068404	-1.759079126	-0.795908057
H	-5.448244392	0.387930030	-1.981802141
H	-3.525260255	1.865826136	-1.610285115
C	-1.406582100	1.475419107	-0.029545003
O	-1.663217122	2.657779191	0.144988010
H	1.952619143	-1.651854120	-0.799118057
H	3.137439224	2.229989160	0.542275037
O	4.017833287	-0.033045002	-0.102493008
C	4.475770324	-1.300170096	-0.486711034
H	5.549843397	-1.269036090	-0.388675027
H	4.216404303	-1.518982110	-1.516799111
H	4.080419292	-2.076090149	0.159543014
H	-0.359437026	-0.953028069	-0.763542053
O	0.771413056	3.202911230	0.670298047
H	-0.168113013	3.355909242	0.554002039
C	3.503101254	5.471436395	1.679003120
O	2.320295168	5.793101416	1.016073072
H	1.851425133	4.993315357	0.814015058
H	3.327489238	4.840390350	2.547661184
H	3.952678285	6.395538461	2.017643147

H	4.216160305	4.967536355	1.028126073
C	-4.313078308	5.540141398	-0.254606018
O	-4.431373321	4.147451301	-0.280759022
H	-3.625640263	3.752352268	0.024730003
H	-5.260806376	5.951580429	-0.574359043
H	-3.538128253	5.898937427	-0.928508064
H	-4.100426293	5.913107428	0.744338051

1.6 angstrom

C	-2.641898191	-0.688497051	0.429537031
C	-3.752655270	-1.499541107	0.229164018
C	-4.757336341	-1.102213079	-0.650544046
C	-4.664405334	0.102864008	-1.309550096
C	-3.566507256	0.932475068	-1.106115078
C	-2.538903184	0.533963038	-0.249418018
C	0.014176002	1.009990073	-0.043392005
C	0.399716030	-0.270286022	-0.444775034
C	1.037692074	1.928530137	0.299011022
C	1.731205127	-0.660330047	-0.474988033
C	2.365406168	1.542770109	0.272594018
C	2.712741197	0.243182018	-0.110929008
H	-1.876119137	-0.992177073	1.119403079
H	-3.837948276	-2.432317176	0.755191053
H	-5.610733405	-1.736459127	-0.803529056
H	-5.443208392	0.414193028	-1.980703140
H	-3.514448253	1.882484133	-1.602275117
C	-1.393315103	1.467305105	-0.024838003
O	-1.633383119	2.653204190	0.161017011
H	1.975942143	-1.655108121	-0.790413059
H	3.136125224	2.240416164	0.536409038
O	4.027220288	-0.021561999	-0.098798006
C	4.492558324	-1.287492094	-0.478239033
H	5.566466400	-1.249982090	-0.380253028
H	4.234594305	-1.511526109	-1.507496106
H	4.101598294	-2.063183146	0.170867010
H	-0.343777026	-0.974877073	-0.758788056
O	0.738223054	3.190702232	0.651386046
H	-0.215546017	3.297563238	0.527856036
C	3.478550250	5.455573391	1.670022119
O	2.299615164	5.780517417	1.002136072
H	1.818621129	4.984308358	0.812727056
H	3.296191235	4.841209347	2.549381185
H	3.939232283	6.380009458	1.992979142
H	4.185773301	4.932582357	1.027469073
C	-4.309177309	5.550321398	-0.254793019
O	-4.409862319	4.155881301	-0.279450022
H	-3.602792257	3.771947273	0.036402002

H	-5.259401379	5.949318429	-0.582752043
H	-3.533326255	5.917391425	-0.923067064
H	-4.109090295	5.927222427	0.745196054

1.5 angstrom

C	-2.640358190	-0.695429051	0.419278030
C	-3.758574271	-1.493941109	0.210102016
C	-4.759605342	-1.076981077	-0.664905048
C	-4.655619335	0.134548009	-1.310472092
C	-3.551083258	0.952672070	-1.096978076
C	-2.527842184	0.534596040	-0.244403015
C	0.029615003	0.990863073	-0.037486001
C	0.421849033	-0.292243020	-0.424499030
C	1.044127076	1.925333139	0.287941021
C	1.755649126	-0.668434047	-0.455692034
C	2.376351173	1.552256114	0.260319021
C	2.731290198	0.250585018	-0.107648009
H	-1.877543137	-1.013553071	1.105823078
H	-3.851822277	-2.431966173	0.725458050
H	-5.619200405	-1.701133122	-0.824686060
H	-5.431213389	0.459661033	-1.978779142
H	-3.491129254	1.908054137	-1.581521114
C	-1.372969100	1.452188104	-0.011916003
O	-1.597979114	2.640345188	0.190936015
H	2.009825146	-1.664517120	-0.759361055
H	3.142833229	2.260067161	0.509008039
O	4.047748291	-0.003969999	-0.098685006
C	4.522253328	-1.271109089	-0.462157035
H	5.596089403	-1.222910085	-0.368468029
H	4.262942304	-1.511746109	-1.487371109
H	4.140366300	-2.041139146	0.199067014
H	-0.317108022	-1.007249073	-0.725514052
O	0.712914051	3.182653229	0.616791046
H	-0.258404019	3.240121233	0.500509034
C	3.433760248	5.447940390	1.655922117
O	2.244380162	5.774978418	1.008484072
H	1.765348125	4.978418356	0.814728061
H	3.266104233	4.829212349	2.535141184
H	3.899544280	6.370837456	1.976058144
H	4.131210296	4.928573352	1.000070074
C	-4.304882311	5.560907398	-0.272051019
O	-4.370646316	4.164113299	-0.293476019
H	-3.565591255	3.799705271	0.049301005
H	-5.256265379	5.934338427	-0.625277044
H	-3.521793255	5.944469430	-0.922229064
H	-4.139547298	5.945965430	0.731022052

1.4 angstrom

C	-2.637008191	-0.696785051	0.414959028
C	-3.762973269	-1.481955107	0.197107016
C	-4.758847343	-1.046200074	-0.674765049
C	-4.643015333	0.170780014	-1.307851093
C	-3.531461254	0.976806072	-1.084836078
C	-2.513262181	0.539267040	-0.235945017
C	0.048655001	0.972078069	-0.031403003
C	0.444411034	-0.313158021	-0.409743029
C	1.055525077	1.920421136	0.277905021
C	1.779495128	-0.677152046	-0.445703031
C	2.391588171	1.557680112	0.244690020
C	2.751246197	0.254510020	-0.112556006
H	-1.877945137	-1.028581076	1.099082080
H	-3.865848279	-2.424035176	0.703128050
H	-5.624219402	-1.660313119	-0.842009058
H	-5.414811392	0.509790036	-1.973587140
H	-3.462850249	1.936834140	-1.558716114
C	-1.347699098	1.438457102	0.005076000
O	-1.556444113	2.628976190	0.224170019
H	2.041081148	-1.673722121	-0.741258055
H	3.155309228	2.272818163	0.480386032
O	4.068931293	0.007126001	-0.109483010
C	4.548894328	-1.262135090	-0.458146036
H	5.622837403	-1.206611087	-0.370004024
H	4.286549309	-1.518017108	-1.478874105
H	4.174422301	-2.025321143	0.215124014
H	-0.291636022	-1.036290077	-0.698582053
O	0.696823052	3.170305227	0.590672043
H	-0.296201022	3.181347230	0.482406034
C	3.383500242	5.456905394	1.636677115
O	2.175800156	5.770606414	1.018045072
H	1.707672123	4.968035359	0.820404058
H	3.245009233	4.827085347	2.513064179
H	3.841280278	6.384179459	1.956157143
H	4.075417291	4.955428357	0.961336067
C	-4.308581312	5.578373401	-0.295614022
O	-4.333238310	4.179920299	-0.311598022
H	-3.530939253	3.839738276	0.060923002
H	-5.258149377	5.921740426	-0.682061049
H	-3.515722253	5.981321429	-0.921576065
H	-4.188107301	5.972293432	0.710199049

1.3 angstrom

C	-2.634276191	-0.693781050	0.413539029
C	-3.763747270	-1.473471105	0.194000015
C	-4.757605343	-1.030251074	-0.676575047

C	-4.637406335	0.188477013	-1.305516093
C	-3.523139254	0.990367070	-1.080488077
C	-2.506497179	0.544392037	-0.234014017
C	0.056747005	0.958115071	-0.031361002
C	0.455580034	-0.328004025	-0.408772031
C	1.055681073	1.916778137	0.277221022
C	1.791032129	-0.682859048	-0.443382033
C	2.394995173	1.558475111	0.244914015
C	2.758491200	0.256184020	-0.110303008
H	-1.875446134	-1.030067074	1.095587081
H	-3.870688277	-2.416617175	0.697092048
H	-5.625434404	-1.640243119	-0.846213059
H	-5.408019391	0.532515040	-1.969954143
H	-3.451201248	1.951816143	-1.551124114
C	-1.332052094	1.428730105	0.007934002
O	-1.525724109	2.623211190	0.234833020
H	2.059503147	-1.677881121	-0.737758055
H	3.156412229	2.276276162	0.479438033
O	4.076729291	0.012581999	-0.106790006
C	4.561570329	-1.255565090	-0.452603031
H	5.635317408	-1.195930084	-0.364057024
H	4.300923308	-1.514535111	-1.472917104
H	4.189791302	-2.018780148	0.222034016
H	-0.277462020	-1.054763078	-0.696886050
O	0.673019050	3.155550226	0.582633041
H	-0.349528024	3.126677225	0.465244033
C	3.364010242	5.444108390	1.625486117
O	2.155608154	5.754716412	1.007094072
H	1.684554120	4.951457358	0.816444061
H	3.227102234	4.820393345	2.506818178
H	3.823502277	6.373242461	1.937565140
H	4.054635294	4.937165354	0.952399068
C	-4.307972309	5.598735401	-0.300659023
O	-4.316628310	4.199474304	-0.309029020
H	-3.514874252	3.871986280	0.075462004
H	-5.257778376	5.929044426	-0.697749048
H	-3.513781252	6.006773431	-0.921410067
H	-4.201232305	5.999075431	0.704129053

1.2 angstrom

C	-2.617470189	-0.699280048	0.398341026
C	-3.761700269	-1.460721103	0.178613012
C	-4.753193344	-0.994164070	-0.679339051
C	-4.621736333	0.230491014	-1.295115093
C	-3.496013253	1.019441073	-1.068193078
C	-2.478556176	0.547588040	-0.235110017
C	0.085728006	0.943945070	-0.024270000

C	0.487915034	-0.345240026	-0.396912031
C	1.076214077	1.915865137	0.276077020
C	1.823073134	-0.689425048	-0.434630034
C	2.420750176	1.561080113	0.238449015
C	2.787112201	0.260616017	-0.109619009
H	-1.858386132	-1.054333074	1.070036075
H	-3.876580279	-2.407996174	0.672003046
H	-5.630869403	-1.589664114	-0.850532061
H	-5.392398386	0.591076043	-1.950445140
H	-3.417806248	1.986691141	-1.525464108
C	-1.292971095	1.411391099	0.015828999
O	-1.480109104	2.606882188	0.257578021
H	2.098966149	-1.683568120	-0.724866054
H	3.180004231	2.283709165	0.464649031
O	4.106230293	0.020160002	-0.109638006
C	4.594245331	-1.249680088	-0.443284034
H	5.667841409	-1.185754085	-0.356263027
H	4.333994314	-1.519934111	-1.460828108
H	4.225790304	-2.007609147	0.239178020
H	-0.242120018	-1.077552075	-0.678596049
O	0.676685047	3.143278224	0.571431042
H	-0.393381027	3.075665221	0.455732035
C	3.349699241	5.417357390	1.619863117
O	2.140813152	5.706299408	0.993561073
H	1.678255122	4.895085354	0.810982057
H	3.216652233	4.807940344	2.511958183
H	3.801504273	6.355511456	1.916698136
H	4.046954292	4.904461354	0.957928070
C	-4.299183310	5.645275407	-0.315960025
O	-4.288534311	4.245349304	-0.311772021
H	-3.493716253	3.933341281	0.098414009
H	-5.250623376	5.957977431	-0.722574049
H	-3.506048253	6.058024438	-0.934648066
H	-4.205424304	6.055504438	0.685919047

1.1 angstrom

C	-2.608264187	-0.689907049	0.409843027
C	-3.753989268	-1.439435101	0.170440012
C	-4.740870340	-0.952088070	-0.680900050
C	-4.597308331	0.283330019	-1.274137094
C	-3.465772249	1.053349074	-1.030290075
C	-2.455200176	0.558989042	-0.202975015
C	0.090787009	0.957648067	-0.026360002
C	0.493807036	-0.346482026	-0.403005031
C	1.090589076	1.945658139	0.262586017
C	1.811236132	-0.685636049	-0.451176030
C	2.441156177	1.573025115	0.212577015

C	2.793993199	0.277795021	-0.132953011
H	-1.858108134	-1.058618076	1.084405079
H	-3.878432278	-2.394031170	0.647376047
H	-5.622382406	-1.538212110	-0.864194063
H	-5.362386384	0.664040050	-1.924648141
H	-3.376786242	2.026483148	-1.472211107
C	-1.255974091	1.406083102	0.041359002
O	-1.462086105	2.612659190	0.308560021
H	2.090460148	-1.677478121	-0.745784055
H	3.205443232	2.292690166	0.430886031
O	4.106858294	0.018549001	-0.149884011
C	4.585208328	-1.259019093	-0.472947033
H	5.659326407	-1.199131088	-0.390932026
H	4.320325311	-1.538066110	-1.486649105
H	4.216539302	-2.007559145	0.219288015
H	-0.241616019	-1.076624078	-0.675930049
O	0.702395050	3.147843225	0.555255040
H	-0.469352036	3.060000220	0.464658033
C	3.324132238	5.428214393	1.592881115
O	2.076138151	5.700285409	1.042431073
H	1.638823120	4.879528353	0.836990061
H	3.260152232	4.764443345	2.453834179
H	3.754300270	6.365775458	1.922579137
H	4.008003290	4.981929357	0.870749061
C	-4.273287307	5.675099408	-0.387662028
O	-4.208112302	4.276566306	-0.363946024
H	-3.426798244	4.000164286	0.095083007
H	-5.200356374	5.944825429	-0.873517065
H	-3.449880247	6.112734439	-0.946506071
H	-4.277069310	6.098718438	0.613124044

1.0 angstrom

C	-2.606720186	-0.692861049	0.434950032
C	-3.730512266	-1.477287108	0.190384014
C	-4.718702338	-1.028313074	-0.679600047
C	-4.589352331	0.204864013	-1.293868092
C	-3.479792250	0.993171069	-1.054313076
C	-2.464652176	0.544802038	-0.200539016
C	0.029878004	1.055384078	-0.024110003
C	0.435770030	-0.273240022	-0.428969033
C	1.095451077	2.034102147	0.271680018
C	1.711300125	-0.643688046	-0.487821036
C	2.470807180	1.576551113	0.215186018
C	2.773171201	0.301555021	-0.142105010
H	-1.861090132	-1.030199072	1.131436083
H	-3.839935278	-2.425583173	0.683606051
H	-5.586712404	-1.634266115	-0.861632062

H	-5.354937383	0.560021038	-1.958737141
H	-3.402455244	1.956190142	-1.520155111
C	-1.295752096	1.427793101	0.039858001
O	-1.664579118	2.674808195	0.311061023
H	1.962926140	-1.633869116	-0.811785057
H	3.247617235	2.277178166	0.452275031
O	4.073220296	-0.041077003	-0.175447013
C	4.478478320	-1.342312095	-0.505173039
H	5.554022400	-1.343367094	-0.418573028
H	4.206779305	-1.601873117	-1.522285108
H	4.069602295	-2.076142152	0.180178011
H	-0.321990021	-0.972507068	-0.718621053
O	0.846011062	3.206158230	0.560407041
H	-0.848345062	3.234252234	0.455241032
C	3.424824244	5.592616403	1.639091116
O	2.147386153	5.879883421	1.161860086
H	1.727392124	5.070402364	0.900895066
H	3.408534247	4.852464350	2.436624176
H	3.840021275	6.508864467	2.037494146
H	4.087264295	5.233692376	0.852928059
C	-4.228666303	5.607933401	-0.391505030
O	-4.347940315	4.215851302	-0.418052032
H	-3.604574262	3.818659273	0.016376004
H	-5.096661367	6.016637432	-0.890315062
H	-3.339034240	5.954176430	-0.913234067
H	-4.206409304	5.996943429	0.623689047

LIIC path connecting Franck-Condon point and S2-PP-ENOL
Coord_1

C	-2.637431189	-0.695595048	0.436158033
C	-3.736978267	-1.523800110	0.243698019
C	-4.750410342	-1.147863083	-0.635095044
C	-4.675607339	0.053070006	-1.303631095
C	-3.587005259	0.897287067	-1.110708078
C	-2.550899183	0.522000039	-0.253248017
C	-0.005549000	1.052874074	-0.040131003
C	0.369371027	-0.227380018	-0.454634034
C	1.038664077	1.944421139	0.317609020
C	1.693231124	-0.646326048	-0.487964036
C	2.357777168	1.530150110	0.286557021
C	2.689447195	0.231993015	-0.111990009
H	-1.867100136	-0.984384070	1.127377082
H	-3.807979275	-2.453741176	0.776626055
H	-5.595569402	-1.795063131	-0.779434055
H	-5.461169393	0.349656026	-1.973727140
H	-3.548627256	1.843053131	-1.616089115
C	-1.427195105	1.488841106	-0.036476003

O	-1.709663126	2.665927193	0.120122008
H	1.916141140	-1.642602117	-0.814793060
H	3.137568227	2.211928161	0.564997040
O	4.000131287	-0.051352006	-0.099748006
C	4.445979322	-1.319964093	-0.493115037
H	5.520039399	-1.300779094	-0.392400028
H	4.186598299	-1.527752112	-1.525463108
H	4.041023289	-2.096791151	0.146030013
H	-0.383459028	-0.916571064	-0.778715057
O	0.819464060	3.219030233	0.705953052
H	-0.100960008	3.438381246	0.605170044
C	3.567884255	5.470021396	1.689361124
O	2.387378174	5.792071415	1.022001074
H	1.924343139	4.991646359	0.810230059
H	3.390906242	4.822152346	2.545209183
H	4.005295289	6.392334462	2.047926146
H	4.290869311	4.984147356	1.035644073
C	-4.311069308	5.532672400	-0.254039016
O	-4.462977321	4.143584296	-0.278974022
H	-3.659670265	3.729799269	0.007872999
H	-5.254252378	5.967519428	-0.556090040
H	-3.540258255	5.873784420	-0.941803066
H	-4.071159293	5.899610424	0.741088051

Coord_2

C	-2.642037190	-0.696405049	0.433993031
C	-3.740956267	-1.524929110	0.239285019
C	-4.754547344	-1.147315083	-0.638434047
C	-4.679952339	0.055460004	-1.303756092
C	-3.591635259	0.899591063	-1.108611080
C	-2.555389183	0.523086038	-0.251834019
C	-0.016450999	1.053092074	-0.039620003
C	0.368100028	-0.231650018	-0.453528033
C	1.032212073	1.947847139	0.309953022
C	1.698780124	-0.647399045	-0.483354034
C	2.359805171	1.533939109	0.278141018
C	2.693423195	0.229839015	-0.114801009
H	-1.871884136	-0.986540071	1.124961081
H	-3.811520275	-2.456149176	0.770139057
H	-5.599505401	-1.794399130	-0.784400055
H	-5.465505392	0.353453027	-1.973278143
H	-3.553659256	1.846678133	-1.611522114
C	-1.431183101	1.488179105	-0.032420002
O	-1.713495126	2.667918191	0.129493012
H	1.921330136	-1.645565118	-0.804879056
H	3.137403225	2.219902158	0.551429041
O	4.005295289	-0.048546001	-0.100282010

C	4.453666320	-1.318061097	-0.487834033
H	5.527729397	-1.296495092	-0.387887029
H	4.193664303	-1.531007108	-1.518986111
H	4.050175293	-2.092427153	0.155235009
H	-0.380559025	-0.923379067	-0.781073054
O	0.815693058	3.221940232	0.690464050
H	-0.107770005	3.437662248	0.597928042
C	3.567807259	5.467010393	1.689573123
O	2.392066171	5.798235419	1.018159073
H	1.925126141	5.001540359	0.801525057
H	3.383179243	4.818668349	2.543446182
H	4.009712289	6.385742458	2.051667148
H	4.290252311	4.977894360	1.037652073
C	-4.305737308	5.530018396	-0.249903019
O	-4.461376322	4.141513297	-0.272445017
H	-3.658615266	3.725729266	0.013578000
H	-5.247367380	5.967081428	-0.553798041
H	-3.533232252	5.867951421	-0.937417065
H	-4.065925291	5.898306425	0.744804055

Coord_3

C	-2.646618192	-0.697218051	0.431818033
C	-3.744964271	-1.525977109	0.234848016
C	-4.758697343	-1.146599080	-0.641775044
C	-4.684237336	0.058020004	-1.303845094
C	-3.596148257	0.901983065	-1.106467082
C	-2.559780185	0.524171036	-0.250393016
C	-0.027223000	1.053151077	-0.039071003
C	0.366953026	-0.236007015	-0.452440034
C	1.025893072	1.951053138	0.302311019
C	1.704424123	-0.648558049	-0.478788034
C	2.361960171	1.537513109	0.269713018
C	2.697510195	0.227496014	-0.117586011
H	-1.876657135	-0.988767071	1.122517081
H	-3.815148272	-2.458480175	0.763601056
H	-5.603496403	-1.793504127	-0.789377057
H	-5.469767396	0.357488024	-1.972776145
H	-3.558517256	1.850394132	-1.606879118
C	-1.435007105	1.487428107	-0.028327001
O	-1.717082122	2.669808195	0.138954008
H	1.926565138	-1.648583117	-0.795033057
H	3.137354228	2.227605158	0.537845040
O	4.010540288	-0.045961002	-0.100831005
C	4.461386323	-1.316354093	-0.482597036
H	5.535448400	-1.292458094	-0.383429029
H	4.200765300	-1.534419110	-1.512531106
H	4.059327292	-2.088235148	0.164366010

H	-0.377550028	-0.930195066	-0.783483055
O	0.811841060	3.224530232	0.674990050
H	-0.114608007	3.436426249	0.590700042
C	3.567001259	5.464332391	1.689639122
O	2.396031175	5.804425417	1.014197075
H	1.925334139	5.011399360	0.792833056
H	3.374856243	4.815680345	2.541618181
H	4.013242288	6.379571458	2.055108150
H	4.288930310	4.971974359	1.039560075
C	-4.300003307	5.527473397	-0.245628018
O	-4.459399321	4.139568296	-0.265789021
H	-3.657191266	3.721763268	0.019379000
H	-5.240075376	5.966763429	-0.551330037
H	-3.525833253	5.862214420	-0.932910068
H	-4.060241292	5.897097424	0.748652052

Coord_4

C	-2.651178192	-0.698036053	0.429631028
C	-3.749007270	-1.526945111	0.230382014
C	-4.762864344	-1.145714084	-0.645122048
C	-4.688464335	0.060754004	-1.303903092
C	-3.600544259	0.904463065	-1.104277082
C	-2.564073183	0.525253040	-0.248927021
C	-0.037863003	1.053049078	-0.038484003
C	0.365928026	-0.240458015	-0.451369032
C	1.019710075	1.954033141	0.294687020
C	1.710162124	-0.649809045	-0.474265034
C	2.364246170	1.540865108	0.261276017
C	2.701711196	0.224959017	-0.120344008
H	-1.881424133	-0.991070071	1.120044082
H	-3.818870277	-2.460735180	0.757006052
H	-5.607549403	-1.792376128	-0.794372057
H	-5.473956395	0.361767026	-1.972224144
H	-3.563198258	1.854204134	-1.602161117
C	-1.438668101	1.486583106	-0.024198000
O	-1.720420124	2.671596195	0.148509012
H	1.931847137	-1.651665119	-0.785258058
H	3.137425228	2.235030161	0.524248037
O	4.015870288	-0.043602004	-0.101395007
C	4.469143321	-1.314851092	-0.477404034
H	5.543200397	-1.288675091	-0.379027025
H	4.207899303	-1.537996110	-1.506102111
H	4.068481291	-2.084226149	0.173422010
H	-0.374433026	-0.937022066	-0.785943057
O	0.807911057	3.226795232	0.659540048
H	-0.121473008	3.434663247	0.583497040
C	3.565465258	5.462007393	1.689557121

O	2.399257171	5.810655416	1.010115070
H	1.924953137	5.021229362	0.784158057
H	3.365942242	4.813205346	2.539725182
H	4.015881290	6.373851459	2.058241149
H	4.286898306	4.966412356	1.041361077
C	-4.293862311	5.525039399	-0.241209018
O	-4.457040323	4.137751297	-0.259004021
H	-3.655395265	3.717900268	0.025277003
H	-5.232370375	5.966568427	-0.548683040
H	-3.518054252	5.856575423	-0.928277068
H	-4.054102291	5.895982427	0.752635053

Coord_5

C	-2.655719189	-0.698861051	0.427429032
C	-3.753089269	-1.527832108	0.225883018
C	-4.767050342	-1.144658084	-0.648481048
C	-4.692630336	0.063664002	-1.303932096
C	-3.604821260	0.907034068	-1.102043081
C	-2.568269183	0.526331037	-0.247435016
C	-0.048371002	1.052782076	-0.037854001
C	0.365027027	-0.245007018	-0.450313032
C	1.013663072	1.956784138	0.287084018
C	1.715995123	-0.651158045	-0.469786035
C	2.366664171	1.543991112	0.252833021
C	2.706026197	0.222220016	-0.123075007
H	-1.886188136	-0.993453073	1.117541079
H	-3.822691276	-2.462915178	0.750348055
H	-5.611666402	-1.791010131	-0.799391059
H	-5.478069393	0.366295026	-1.971627142
H	-3.567699254	1.858108134	-1.597367115
C	-1.442163105	1.485641107	-0.020030999
O	-1.723505122	2.673276195	0.158161009
H	1.937174142	-1.654815121	-0.775555053
H	3.137618224	2.242171159	0.510641038
O	4.021284290	-0.041477003	-0.101974006
C	4.476934323	-1.313560095	-0.472257034
H	5.550983398	-1.285156094	-0.374682025
H	4.215067305	-1.541742108	-1.499701109
H	4.077636296	-2.080408151	0.182399016
H	-0.371208029	-0.943867069	-0.788453056
O	0.803902057	3.228730232	0.644120046
H	-0.128366007	3.432361247	0.576331043
C	3.563191257	5.460055396	1.689320123
O	2.401726175	5.816938417	1.005911075
H	1.923963136	5.031036361	0.775504057
H	3.356443240	4.811262344	2.537767184
H	4.017624288	6.368607456	2.061056150

H	4.284150310	4.961231357	1.043049073
C	-4.287304307	5.522715395	-0.236643017
O	-4.454295322	4.136063296	-0.252086018
H	-3.653221262	3.714139268	0.031277000
H	-5.224242377	5.966499428	-0.545852037
H	-3.509883253	5.851035424	-0.923513065
H	-4.047500292	5.894959427	0.756760053

Coord_6

C	-2.660245189	-0.699695050	0.425210033
C	-3.757214270	-1.528639108	0.221346017
C	-4.771256343	-1.143427080	-0.651856046
C	-4.696737338	0.066755006	-1.303937092
C	-3.608977260	0.909696067	-1.099764078
C	-2.572365184	0.527403039	-0.245918018
C	-0.058746004	1.052346077	-0.037179004
C	0.364249026	-0.249658015	-0.449272035
C	1.007757072	1.959299143	0.279507020
C	1.721923125	-0.652613049	-0.465350032
C	2.369215170	1.546883113	0.244387018
C	2.710455193	0.219276018	-0.125777008
H	-1.890954134	-0.995919070	1.115003081
H	-3.826619274	-2.465021177	0.743621053
H	-5.615849406	-1.789400130	-0.804440056
H	-5.482102396	0.371076026	-1.970988139
H	-3.572013255	1.862109132	-1.592499113
C	-1.445492107	1.484597109	-0.015825003
O	-1.726333124	2.674844195	0.167911010
H	1.942546137	-1.658042118	-0.765925054
H	3.137936228	2.249020163	0.497031038
O	4.026785288	-0.039593005	-0.102568008
C	4.484761321	-1.312488094	-0.467157035
H	5.558800399	-1.281908094	-0.370395028
H	4.222268301	-1.545665111	-1.493329105
H	4.086793295	-2.076789150	0.191296014
H	-0.367876028	-0.950733070	-0.791013056
O	0.799814057	3.230330231	0.628737043
H	-0.135284010	3.429509246	0.569213043
C	3.560174258	5.458499392	1.688923124
O	2.403420172	5.823285422	1.001583072
H	1.922349141	5.040826362	0.766874054
H	3.346363239	4.809868349	2.535744181
H	4.018464288	6.363868456	2.063542150
H	4.280678309	4.956453357	1.044616078
C	-4.280322305	5.520500397	-0.231923016
O	-4.451156322	4.134505297	-0.245034017
H	-3.650665261	3.710479267	0.037382002

H	-5.215681374	5.966557431	-0.542834038
H	-3.501313254	5.845592423	-0.918611069
H	-4.040428293	5.894026424	0.761032054

Coord_7

C	-2.664758193	-0.700540051	0.422970031
C	-3.761386271	-1.529365108	0.216765014
C	-4.775484342	-1.142018083	-0.655254046
C	-4.700780337	0.070029005	-1.303921095
C	-3.613009262	0.912451065	-1.097444081
C	-2.576363187	0.528467040	-0.244378017
C	-0.068985007	1.051736078	-0.036457005
C	0.363593026	-0.254417018	-0.448245034
C	1.001992073	1.961573139	0.271961021
C	1.727944125	-0.654179049	-0.460959031
C	2.371901168	1.549535111	0.235941016
C	2.714999196	0.216118015	-0.128450009
H	-1.895726138	-0.998475071	1.112428078
H	-3.830658277	-2.467052180	0.736818051
H	-5.620102403	-1.787543131	-0.809528058
H	-5.486055393	0.376119027	-1.970311142
H	-3.576137255	1.866208134	-1.587554115
C	-1.448653104	1.483448107	-0.011579001
O	-1.728899126	2.676296194	0.177763015
H	1.947962140	-1.661353122	-0.756370055
H	3.138381223	2.255571160	0.483420033
O	4.032372289	-0.037959001	-0.103176006
C	4.492623323	-1.311643093	-0.462106033
H	5.566649400	-1.278941092	-0.366168029
H	4.229501302	-1.549772114	-1.486989107
H	4.095953295	-2.073380148	0.200111012
H	-0.364440027	-0.957625069	-0.793620059
O	0.795649057	3.231588234	0.613399047
H	-0.142227012	3.426096248	0.562155041
C	3.556406257	5.457357391	1.688362122
O	2.404320175	5.829709422	0.997128071
H	1.920090136	5.050601361	0.758271056
H	3.335703239	4.809043345	2.533655180
H	4.018395289	6.359663455	2.065689149
H	4.276477309	4.952102356	1.046054074
C	-4.272906310	5.518396399	-0.227045017
O	-4.447617322	4.133076296	-0.237843017
H	-3.647720263	3.706918269	0.043596003
H	-5.206677375	5.966745432	-0.539624039
H	-3.492330253	5.840245420	-0.913563067
H	-4.032877288	5.893182423	0.765459055

Coord_8

C	-2.669260195	-0.701398048	0.420707031
C	-3.765609270	-1.530010111	0.212135015
C	-4.779737345	-1.140427085	-0.658679045
C	-4.704761338	0.073491004	-1.303888095
C	-3.616914262	0.915300065	-1.095082077
C	-2.580260186	0.529522040	-0.242816018
C	-0.079088006	1.050948075	-0.035684004
C	0.363060028	-0.259289020	-0.447232030
C	0.996372073	1.963601142	0.264449017
C	1.734061123	-0.655865045	-0.456611035
C	2.374725170	1.551940111	0.227499014
C	2.719658194	0.212740018	-0.131092011
H	-1.900508138	-1.001122073	1.109814080
H	-3.834817277	-2.469008178	0.729931053
H	-5.624428406	-1.785432126	-0.814662056
H	-5.489923392	0.381427029	-1.969599144
H	-3.580065259	1.870408134	-1.582534112
C	-1.451644104	1.482188109	-0.007291999
O	-1.731199126	2.677626191	0.187722015
H	1.953422143	-1.664755117	-0.746892051
H	3.138957228	2.261816161	0.469813034
O	4.038046291	-0.036582002	-0.103796006
C	4.500521325	-1.311035094	-0.457105033
H	5.574532400	-1.276264090	-0.362002028
H	4.236765303	-1.554070113	-1.480683108
H	4.105113295	-2.070191151	0.208843013
H	-0.360897026	-0.964548067	-0.796275057
O	0.791405055	3.232499234	0.598113042
H	-0.149191011	3.422108247	0.555168038
C	3.551879257	5.456655395	1.687630122
O	2.404405172	5.836222419	0.992544073
H	1.917166140	5.060366364	0.749696056
H	3.324466239	4.808806348	2.531502180
H	4.017405288	6.356023457	2.067483150
H	4.271538307	4.948204357	1.047356073
C	-4.265045307	5.516401395	-0.222002016
O	-4.443670321	4.131777299	-0.230510017
H	-3.644382261	3.703456264	0.049923005
H	-5.197217374	5.967065431	-0.536216037
H	-3.482924249	5.834994421	-0.908362064
H	-4.024839292	5.892423424	0.770048054

Coord_9

C	-2.673755190	-0.702270053	0.418417032
C	-3.769886271	-1.530572108	0.207450013
C	-4.784016347	-1.138651081	-0.662139050

C	-4.708676339	0.077146005	-1.303840094
C	-3.620690260	0.918244068	-1.092680078
C	-2.584056186	0.530567038	-0.241232016
C	-0.089054006	1.049978077	-0.034858001
C	0.362650027	-0.264279019	-0.446230033
C	0.990900073	1.965378141	0.256976018
C	1.740272124	-0.657676048	-0.452308030
C	2.377689171	1.554090110	0.219065014
C	2.724434194	0.209135013	-0.133703009
H	-1.905305135	-1.003867075	1.107157081
H	-3.839100274	-2.470890176	0.722954052
H	-5.628829404	-1.783062127	-0.819849057
H	-5.493703395	0.387010029	-1.968855142
H	-3.583791259	1.874710133	-1.577436114
C	-1.454464106	1.480815106	-0.002961001
O	-1.733228124	2.678829190	0.197789014
H	1.958925142	-1.668255122	-0.737491053
H	3.139667225	2.267747163	0.456217031
O	4.043810291	-0.035471005	-0.104428008
C	4.508455322	-1.310673095	-0.452154035
H	5.582449399	-1.273888090	-0.357897025
H	4.244059307	-1.558566114	-1.474411109
H	4.114276296	-2.067232151	0.217488018
H	-0.357251027	-0.971508071	-0.798978058
O	0.787084058	3.233056235	0.582887041
H	-0.156175013	3.417533245	0.548262037
C	3.546584256	5.456413391	1.686721122
O	2.403653174	5.842835420	0.987825072
H	1.913558136	5.070126366	0.741152055
H	3.312653241	4.809178344	2.529282181
H	4.015485290	6.352978460	2.068911151
H	4.265852308	4.944785353	1.048514077
C	-4.256730308	5.514516397	-0.216788017
O	-4.439307318	4.130608298	-0.223030017
H	-3.640644264	3.700089268	0.056367003
H	-5.187290374	5.967518428	-0.532605037
H	-3.473083251	5.829839419	-0.903000065
H	-4.016303287	5.891747426	0.774806056

Coord_10

C	-2.667068194	-0.714328050	0.410641032
C	-3.757864269	-1.547831113	0.192596012
C	-4.769697345	-1.159181084	-0.680955047
C	-4.696870337	0.058379003	-1.319676093
C	-3.613924257	0.904241065	-1.101527080
C	-2.579547188	0.520368035	-0.245603020
C	-0.094308006	1.050139074	-0.028311004

C	0.375477029	-0.266072019	-0.436306033
C	0.984178072	1.973821143	0.259740017
C	1.761616129	-0.649401049	-0.432109033
C	2.381596172	1.569829112	0.227910016
C	2.738523199	0.220639015	-0.116264009
H	-1.900786136	-1.013529073	1.102945079
H	-3.824953276	-2.489420180	0.706164051
H	-5.610683403	-1.807244130	-0.843998061
H	-5.480053395	0.365837028	-1.988014142
H	-3.579336259	1.861877135	-1.584113114
C	-1.454820104	1.473895108	0.000166998
O	-1.739661125	2.673231194	0.204435015
H	1.985899142	-1.660755120	-0.710380049
H	3.136601225	2.291159166	0.463017033
O	4.059871292	-0.012688004	-0.078477007
C	4.534631328	-1.286536093	-0.417397033
H	5.607935401	-1.242371092	-0.318830023
H	4.275798306	-1.541329112	-1.439392106
H	4.142147299	-2.041921148	0.254583020
H	-0.335112024	-0.979014069	-0.795700059
O	0.773445054	3.239391233	0.575941039
H	-0.173157014	3.413760243	0.544947038
C	3.514717255	5.477356396	1.705438121
O	2.377722171	5.864048421	0.996966074
H	1.889982136	5.091735367	0.744862053
H	3.273620238	4.830331347	2.546140181
H	3.980506288	6.373894460	2.091349150
H	4.239245302	4.965677356	1.073222077
C	-4.264641307	5.493194396	-0.229305017
O	-4.444301322	4.109109298	-0.233131016
H	-3.645494263	3.680550266	0.049402004
H	-5.194283372	5.943687428	-0.551544042
H	-3.477735248	5.808620417	-0.911813067
H	-4.030641292	5.873551423	0.762688056

LIIC path connecting S2-PP-ENOL and S1-NP-ENOL

Coord_1

C	-2.667068194	-0.714328050	0.410641032
C	-3.757864269	-1.547831113	0.192596012
C	-4.769697345	-1.159181084	-0.680955047
C	-4.696870337	0.058379003	-1.319676093
C	-3.613924257	0.904241065	-1.101527080
C	-2.579547188	0.520368035	-0.245603020
C	-0.094308006	1.050139074	-0.028311004
C	0.375477029	-0.266072019	-0.436306033
C	0.984178072	1.973821143	0.259740017
C	1.761616129	-0.649401049	-0.432109033

C	2.381596172	1.569829112	0.227910016
C	2.738523199	0.220639015	-0.116264009
H	-1.900786136	-1.013529073	1.102945079
H	-3.824953276	-2.489420180	0.706164051
H	-5.610683403	-1.807244130	-0.843998061
H	-5.480053395	0.365837028	-1.988014142
H	-3.579336259	1.861877135	-1.584113114
C	-1.454820104	1.473895108	0.000166998
O	-1.739661125	2.673231194	0.204435015
H	1.985899142	-1.660755120	-0.710380049
H	3.136601225	2.291159166	0.463017033
O	4.059871292	-0.012688004	-0.078477007
C	4.534631328	-1.286536093	-0.417397033
H	5.607935401	-1.242371092	-0.318830023
H	4.275798306	-1.541329112	-1.439392106
H	4.142147299	-2.041921148	0.254583020
H	-0.335112024	-0.979014069	-0.795700059
O	0.773445054	3.239391233	0.575941039
H	-0.173157014	3.413760243	0.544947038
C	3.514717255	5.477356396	1.705438121
O	2.377722171	5.864048421	0.996966074
H	1.889982136	5.091735367	0.744862053
H	3.273620238	4.830331347	2.546140181
H	3.980506288	6.373894460	2.091349150
H	4.239245302	4.965677356	1.073222077
C	-4.264641307	5.493194396	-0.229305017
O	-4.444301322	4.109109298	-0.233131016
H	-3.645494263	3.680550266	0.049402004
H	-5.194283372	5.943687428	-0.551544042
H	-3.477735248	5.808620417	-0.911813067
H	-4.030641292	5.873551423	0.762688056

Coord_2

C	-2.653220192	-0.736787052	0.394519028
C	-3.750213271	-1.564467112	0.183846014
C	-4.779252344	-1.159140083	-0.660840046
C	-4.716503342	0.072641008	-1.279100094
C	-3.629919259	0.910820066	-1.069159075
C	-2.575382187	0.509562035	-0.241843020
C	-0.078955008	1.035877075	-0.035784003
C	0.390301030	-0.272222022	-0.449394031
C	0.989946072	1.958355138	0.274370021
C	1.772277129	-0.651568046	-0.444595034
C	2.380721172	1.562305111	0.245109017
C	2.744728199	0.222886018	-0.113895010
H	-1.874263137	-1.049431077	1.066086079
H	-3.808019276	-2.515003180	0.681853051

H	-5.624758406	-1.802464130	-0.818962061
H	-5.512587398	0.392771028	-1.925855141
H	-3.603627262	1.875966136	-1.537205112
C	-1.445355103	1.451987106	-0.013811002
O	-1.730990122	2.671579192	0.157868009
H	2.003319144	-1.658307119	-0.733721052
H	3.133016223	2.281595166	0.495807035
O	4.066742293	-0.007857002	-0.075064004
C	4.546616325	-1.276924091	-0.423883031
H	5.619394406	-1.230456089	-0.320189024
H	4.293482309	-1.523190112	-1.449413104
H	4.153903300	-2.040088147	0.239153016
H	-0.319168024	-0.983766070	-0.814495059
O	0.772900055	3.223296233	0.608782044
H	-0.173602010	3.391116246	0.613930044
C	3.519704254	5.464311394	1.709929122
O	2.368629170	5.846111419	1.021763071
H	1.885514134	5.071105365	0.768595055
H	3.297068235	4.809551345	2.549748185
H	3.983904289	6.362178460	2.094811149
H	4.238495305	4.962949357	1.063185077
C	-4.291214308	5.523832399	-0.278447020
O	-4.448730319	4.138271298	-0.218289018
H	-3.645303262	3.733370268	0.085955007
H	-5.228183377	5.943479429	-0.620135044
H	-3.509750255	5.819549420	-0.975669071
H	-4.063102294	5.952927429	0.694744052

Coord_3

C	-2.639286188	-0.756785057	0.378455027
C	-3.742828269	-1.578077112	0.175407012
C	-4.787716343	-1.156364083	-0.640588047
C	-4.733404342	0.088845008	-1.238710090
C	-3.642911264	0.918880065	-1.037203077
C	-2.569508182	0.500503034	-0.238524015
C	-0.061987003	1.021248076	-0.043039002
C	0.405605027	-0.279036021	-0.462497031
C	0.997990074	1.941253140	0.289188022
C	1.783088130	-0.655590047	-0.457196035
C	2.381746172	1.551914112	0.262409017
C	2.751715197	0.222218016	-0.111435008
H	-1.848658134	-1.082674077	1.029420076
H	-3.792637273	-2.536933184	0.658119049
H	-5.638039406	-1.794494128	-0.793595055
H	-5.541384398	0.421436031	-1.864028135
H	-3.623747258	1.891001135	-1.491066105
C	-1.433870104	1.430712101	-0.027753002

O	-1.718585123	2.670148191	0.109471009
H	2.020053147	-1.657699121	-0.757275054
H	3.131854224	2.268256163	0.528713039
O	4.074200295	-0.007043000	-0.071632004
C	4.558142330	-1.271565092	-0.430515030
H	5.630409406	-1.223761087	-0.321710022
H	4.310456309	-1.508870110	-1.459505106
H	4.164643301	-2.042202146	0.223387016
H	-0.303368019	-0.988439071	-0.833444060
O	0.774667057	3.205203229	0.641862046
H	-0.170435011	3.365850244	0.682771051
C	3.523485251	5.453865392	1.714822122
O	2.358117170	5.828363417	1.046929074
H	1.880912133	5.049888364	0.792784059
H	3.320394241	4.791458346	2.553611184
H	3.984537285	6.353946457	2.098466150
H	4.237105304	4.963850355	1.053925078
C	-4.326623309	5.553084401	-0.326016022
O	-4.445176322	4.167603302	-0.203513013
H	-3.630562262	3.796827272	0.114544009
H	-5.277504379	5.930730427	-0.677760050
H	-3.558915256	5.838510423	-1.042348077
H	-4.103408297	6.030658433	0.625374047

Coord_4

C	-2.625435190	-0.774559057	0.362234024
C	-3.735656271	-1.589184114	0.167117012
C	-4.794935348	-1.151845084	-0.620870045
C	-4.747535343	0.105809007	-1.199753088
C	-3.653080262	0.927524065	-1.006969075
C	-2.562210182	0.492767034	-0.236429018
C	-0.043803001	1.006152073	-0.050510005
C	0.421198028	-0.286730020	-0.475470034
C	1.007759073	1.922638140	0.303636021
C	1.793890130	-0.661566046	-0.469338034
C	2.384172170	1.538895108	0.279685020
C	2.759191201	0.218748016	-0.108434006
H	-1.824224131	-1.113122078	0.993121072
H	-3.778668274	-2.555586185	0.635242044
H	-5.650201407	-1.784547130	-0.768521055
H	-5.566329401	0.450290034	-1.804174129
H	-3.639975262	1.905940137	-1.447450105
C	-1.420816100	1.409854104	-0.042560001
O	-1.702967123	2.668623192	0.057681003
H	2.036098145	-1.659134117	-0.780042058
H	3.132495227	2.251544163	0.561498041
O	4.081967294	-0.010014002	-0.067368005

C	4.569117328	-1.270334093	-0.435906033
H	5.640865408	-1.222037086	-0.321798025
H	4.326887310	-1.498660106	-1.468244104
H	4.174182298	-2.047923145	0.208876013
H	-0.287768022	-0.993442071	-0.852286061
O	0.778057056	3.185370232	0.674094047
H	-0.164390013	3.338244242	0.750056055
C	3.525122256	5.446521391	1.719057122
O	2.345476168	5.811086420	1.070960077
H	1.875520134	5.028326364	0.816055057
H	3.342436241	4.776930346	2.556850183
H	3.981381288	6.349790458	2.101083149
H	4.234253304	4.968595355	1.044725078
C	-4.368434313	5.582071403	-0.368723029
O	-4.433307321	4.198993303	-0.189474015
H	-3.601856259	3.870090280	0.131059011
H	-5.338655382	5.909761424	-0.717370052
H	-3.624251263	5.865902420	-1.109897082
H	-4.147003300	6.104943441	0.558859039

Coord_5

C	-2.611816189	-0.790674055	0.345734024
C	-3.728584267	-1.598710114	0.158908012
C	-4.800811348	-1.146991084	-0.602229041
C	-4.759064343	0.121996010	-1.163309085
C	-3.660855263	0.935564066	-0.979594069
C	-2.553909185	0.485654034	-0.236208018
C	-0.024967001	0.990384072	-0.058558003
C	0.436810032	-0.295575022	-0.488182036
C	1.018466075	1.902630139	0.317217022
C	1.804478131	-0.669537048	-0.480542034
C	2.387286171	1.523594112	0.296784022
C	2.766745201	0.212724015	-0.104551010
H	-1.801113130	-1.140951081	0.957434068
H	-3.765792270	-2.571776183	0.613562044
H	-5.660944409	-1.774302126	-0.744239053
H	-5.587603401	0.477418036	-1.747737127
H	-3.652951265	1.919483138	-1.407901101
C	-1.406824104	1.388976098	-0.058978006
O	-1.684892122	2.666362192	0.001145002
H	2.051472146	-1.662742122	-0.801176059
H	3.134051225	2.232036161	0.593898045
O	4.089659293	-0.016299003	-0.061633004
C	4.579435332	-1.272819094	-0.438922032
H	5.650626405	-1.224657090	-0.319156022
H	4.342897314	-1.492543108	-1.474465106
H	4.182421302	-2.056695147	0.196951014

H	-0.272451018	-0.999283071	-0.870778065
O	0.782039057	3.164039229	0.704509049
H	-0.156583014	3.308535236	0.814555057
C	3.523184255	5.442920393	1.721621124
O	2.329432170	5.794650418	1.092463078
H	1.868186135	5.006724360	0.837156058
H	3.361639242	4.766943342	2.558644184
H	3.972854284	6.350461454	2.101479153
H	4.228649306	4.977615356	1.034842073
C	-4.412820319	5.612443404	-0.403484031
O	-4.412587317	4.234401304	-0.177407011
H	-3.560205258	3.951720284	0.131637011
H	-5.406015392	5.886201421	-0.733082054
H	-3.703289266	5.901826422	-1.175669083
H	-4.187685303	6.174975446	0.499569036

Coord_6

C	-2.598550186	-0.806033059	0.328952025
C	-3.721428267	-1.607988115	0.150824009
C	-4.805304348	-1.143625083	-0.584997040
C	-4.768392341	0.135509011	-1.130153082
C	-3.666934266	0.941520067	-0.955908069
C	-2.545163182	0.478193032	-0.238295019
C	-0.006195999	0.973656070	-0.067440005
C	0.452095031	-0.305859021	-0.500536038
C	1.029100072	1.881344137	0.329543026
C	1.814591132	-0.679449051	-0.490489037
C	2.390177172	1.506468111	0.313534022
C	2.773850199	0.204560017	-0.099600006
H	-1.779341127	-1.166676086	0.922647067
H	-3.753490269	-2.586774188	0.593460045
H	-5.669991409	-1.765917128	-0.721039054
H	-5.605718403	0.500540034	-1.695786124
H	-3.663715264	1.930081140	-1.373586100
C	-1.392702099	1.367426101	-0.077525007
O	-1.665373122	2.662402190	-0.061147003
H	2.066205150	-1.668515118	-0.820080059
H	3.135386223	2.210478157	0.625637043
O	4.096799296	-0.025150001	-0.054050005
C	4.588974329	-1.278272091	-0.438820033
H	5.659540407	-1.230574091	-0.312948022
H	4.358540312	-1.490104109	-1.477403109
H	4.189366304	-2.067715147	0.188522014
H	-0.257546016	-1.006527074	-0.888725064
O	0.785268054	3.141407228	0.732356055
H	-0.148468012	3.276871238	0.875349061
C	3.515775255	5.443799393	1.721640126

O	2.308175167	5.779464418	1.110312078
H	1.857279135	4.985411360	0.855092061
H	3.376104244	4.762500344	2.558299182
H	3.956847286	6.356804459	2.098628152
H	4.218533305	4.991538359	1.023572074
C	-4.454590322	5.646405407	-0.427705030
O	-4.382447318	4.275592307	-0.169037010
H	-3.507095251	4.039608290	0.112929007
H	-5.472123394	5.866753422	-0.720685051
H	-3.791832273	5.946491427	-1.236341091
H	-4.217639302	6.241078448	0.451305033

Coord_7

C	-2.585721184	-0.821857057	0.312028021
C	-3.713932270	-1.618733117	0.143056010
C	-4.808431347	-1.143955083	-0.569205042
C	-4.776152344	0.144145009	-1.100611079
C	-3.672280263	0.943667066	-0.936294066
C	-2.536665183	0.469169036	-0.242835016
C	0.011645000	0.955628070	-0.077271007
C	0.466616036	-0.317839022	-0.512492036
C	1.038467075	1.858890136	0.340380025
C	1.823912134	-0.691106048	-0.499076038
C	2.391766170	1.488086107	0.329748024
C	2.779877200	0.194853012	-0.093600009
H	-1.758784125	-1.191130086	0.889075062
H	-3.741036268	-2.602294190	0.575349043
H	-5.677098407	-1.761979128	-0.698913048
H	-5.621519402	0.517073039	-1.648813118
H	-3.673701262	1.935992140	-1.345099097
C	-1.379428100	1.344374097	-0.098403007
O	-1.645678119	2.655507190	-0.129701010
H	2.080319149	-1.676247122	-0.836518061
H	3.135169223	2.187761160	0.656447050
O	4.102828297	-0.035528003	-0.044586004
C	4.597601331	-1.285566095	-0.435397034
H	5.667447410	-1.238279091	-0.302961024
H	4.373772314	-1.490446105	-1.476838106
H	4.195136304	-2.079922149	0.183908012
H	-0.243246017	-1.015724074	-0.906009067
O	0.786137058	3.117609223	0.757202054
H	-0.141762008	3.243271235	0.931957067
C	3.500588249	5.449914391	1.718508122
O	2.279418162	5.765924418	1.123814078
H	1.840749130	4.964707358	0.869274064
H	3.383657244	4.764538343	2.555341181
H	3.930786281	6.369658460	2.091816149

H	4.201706305	5.011151361	1.010354073
C	-4.487297323	5.686621407	-0.439622033
O	-4.342453313	4.323889310	-0.166412010
H	-3.444485248	4.130984295	0.072403005
H	-5.527968400	5.858811424	-0.678091050
H	-3.883711281	6.000597430	-1.288181093
H	-4.227685304	6.304507453	0.416574030

Coord_8

C	-2.573365186	-0.839600058	0.295261024
C	-3.705768266	-1.632951115	0.135959008
C	-4.810270349	-1.150451083	-0.554507038
C	-4.783198344	0.145512012	-1.074417075
C	-3.678107266	0.940139068	-0.920547064
C	-2.529226184	0.457213033	-0.249602018
C	0.027568002	0.935970067	-0.087999007
C	0.479849034	-0.331662026	-0.524090035
C	1.045237078	1.835392131	0.349699027
C	1.832061130	-0.704114050	-0.506491034
C	2.390863171	1.469116108	0.345233025
C	2.784114201	0.184407016	-0.086823006
H	-1.739169123	-1.215408088	0.857028061
H	-3.727509270	-2.620399190	0.559640041
H	-5.682059407	-1.765388125	-0.677467050
H	-5.636173405	0.524260039	-1.606559114
H	-3.684710266	1.935383141	-1.322281095
C	-1.368122096	1.318890096	-0.121433007
O	-1.627314118	2.644281192	-0.204376017
H	2.093799151	-1.685456124	-0.850726063
H	3.131946227	2.164883155	0.686087051
O	4.107125296	-0.046098001	-0.033644005
C	4.605157331	-1.293179093	-0.429130030
H	5.674176407	-1.245813088	-0.289777022
H	4.388418316	-1.492122105	-1.473241108
H	4.199961300	-2.091988153	0.182663012
H	-0.229830019	-1.027307076	-0.922624069
O	0.782861054	3.092695224	0.779041056
H	-0.138334008	3.207595232	0.984458070
C	3.475008250	5.461949395	1.712041121
O	2.240514162	5.754339415	1.132903084
H	1.816225130	4.944874356	0.879678064
H	3.381956246	4.773818344	2.549627184
H	3.891748282	6.389741461	2.080826148
H	4.175591301	5.037332363	0.994893070
C	-4.503445326	5.735960412	-0.438665031
O	-4.292459308	4.380018315	-0.171626015
H	-3.374802240	4.222513305	0.008671998

H	-5.563357399	5.869904424	-0.605727046
H	-3.970614288	6.065556435	-1.327581096
H	-4.207778301	6.366916459	0.395932026

Coord_9

C	-2.561485183	-0.860813060	0.279113021
C	-3.696553263	-1.652775121	0.130056009
C	-4.810948346	-1.165662082	-0.540123037
C	-4.790571345	0.137219010	-1.050616074
C	-3.685827264	0.929096065	-0.907771063
C	-2.523751183	0.440946034	-0.257954017
C	0.040496003	0.914441067	-0.099386007
C	0.491179036	-0.347282026	-0.535474040
C	1.048018074	1.811008131	0.357698028
C	1.838586134	-0.717825054	-0.513259036
C	2.386226171	1.450321103	0.359802026
C	2.785787200	0.174232011	-0.079831008
H	-1.720094125	-1.240747089	0.826779062
H	-3.711830267	-2.643340188	0.546715040
H	-5.684705410	-1.779139129	-0.655876046
H	-5.651117408	0.519383035	-1.567865113
H	-3.698844267	1.926505140	-1.304084092
C	-1.360005099	1.290065091	-0.145997013
O	-1.611987118	2.627346187	-0.284269023
H	2.106554153	-1.695316120	-0.863493062
H	3.124235225	2.142898153	0.714352053
O	4.109026296	-0.055261006	-0.022121001
C	4.611448333	-1.299216095	-0.421291031
H	5.679532411	-1.250818089	-0.274891018
H	4.402136315	-1.493109105	-1.467887105
H	4.204148304	-2.102346152	0.183449014
H	-0.217691016	-1.041473077	-0.938709067
O	0.773595055	3.066632218	0.798366059
H	-0.140062010	3.169537227	1.033570074
C	3.436240248	5.480417395	1.702634122
O	2.188613156	5.744867412	1.138320081
H	1.781169127	4.926083356	0.886993061
H	3.368619243	4.790811342	2.541462185
H	3.836608278	6.417518462	2.066139151
H	4.137339295	5.070975363	0.977314072
C	-4.494802321	5.797057418	-0.425767029
O	-4.232712302	4.444071321	-0.186532012
H	-3.300889239	4.310523308	-0.078216006
H	-5.567351401	5.906987424	-0.506800037
H	-4.042034293	6.143423443	-1.351794099
H	-4.147729299	6.429482461	0.387551028

Coord_10

C	-2.545250184	-0.782042057	0.261420017
C	-3.680641263	-1.576236115	0.124998011
C	-4.793766347	-1.102078080	-0.555625041
C	-4.771452345	0.194031014	-1.090514081
C	-3.669317262	0.986644070	-0.961577070
C	-2.504846178	0.510357039	-0.301424023
C	0.064005004	0.980752073	-0.116557009
C	0.518421039	-0.285990018	-0.513839036
C	1.054626074	1.885308135	0.352621028
C	1.859994132	-0.654852046	-0.456712034
C	2.384662172	1.529515108	0.391039026
C	2.796089201	0.250946017	-0.017485001
H	-1.705765121	-1.151708085	0.818526061
H	-3.696498266	-2.558752184	0.560308043
H	-5.667693409	-1.716907123	-0.662223046
H	-5.630975403	0.566026041	-1.616744114
H	-3.682103264	1.975556140	-1.378782102
C	-1.339641099	1.348153095	-0.208036013
O	-1.578431115	2.689718192	-0.442020031
H	2.138669153	-1.637289120	-0.783881054
H	3.114399223	2.227306163	0.753184053
O	4.118146296	0.023148001	0.071238005
C	4.629837332	-1.227782088	-0.292166019
H	5.694462412	-1.175303083	-0.123305009
H	4.444196318	-1.442855105	-1.339113096
H	4.210285305	-2.019571146	0.319160023
H	-0.183955014	-0.988200073	-0.915301065
O	0.761654054	3.150103224	0.768008054
H	-0.147436010	3.247820233	1.015736071
C	3.378310241	5.632120405	1.623142116
O	2.127133153	5.852770421	1.047896077
H	1.741305126	5.018526362	0.813450061
H	3.323218238	4.963406360	2.479633179
H	3.755633268	6.587486474	1.963152141
H	4.091381294	5.219862377	0.911312063
C	-4.420860321	5.961699431	-0.604660044
O	-4.138316299	4.610204333	-0.375253028
H	-3.201185228	4.484727321	-0.331363025
H	-5.496695395	6.068141439	-0.608186042
H	-4.037447289	6.301702454	-1.563657111
H	-4.017269290	6.600492476	0.176879014

LIIC path connecting S1-NP-ENOL and S₁/T₁-ENOL

Coord_1

C	-2.545250184	-0.782042057	0.261420017
C	-3.680641263	-1.576236115	0.124998011

C	-4.793766347	-1.102078080	-0.555625041
C	-4.771452345	0.194031014	-1.090514081
C	-3.669317262	0.986644070	-0.961577070
C	-2.504846178	0.510357039	-0.301424023
C	0.064005004	0.980752073	-0.116557009
C	0.518421039	-0.285990018	-0.513839036
C	1.054626074	1.885308135	0.352621028
C	1.859994132	-0.654852046	-0.456712034
C	2.384662172	1.529515108	0.391039026
C	2.796089201	0.250946017	-0.017485001
H	-1.705765121	-1.151708085	0.818526061
H	-3.696498266	-2.558752184	0.560308043
H	-5.667693409	-1.716907123	-0.662223046
H	-5.630975403	0.566026041	-1.616744114
H	-3.682103264	1.975556140	-1.378782102
C	-1.339641099	1.348153095	-0.208036013
O	-1.578431115	2.689718192	-0.442020031
H	2.138669153	-1.637289120	-0.783881054
H	3.114399223	2.227306163	0.753184053
O	4.118146296	0.023148001	0.071238005
C	4.629837332	-1.227782088	-0.292166019
H	5.694462412	-1.175303083	-0.123305009
H	4.444196318	-1.442855105	-1.339113096
H	4.210285305	-2.019571146	0.319160023
H	-0.183955014	-0.988200073	-0.915301065
O	0.761654054	3.150103224	0.768008054
H	-0.147436010	3.247820233	1.015736071
C	3.378310241	5.632120405	1.623142116
O	2.127133153	5.852770421	1.047896077
H	1.741305126	5.018526362	0.813450061
H	3.323218238	4.963406360	2.479633179
H	3.755633268	6.587486474	1.963152141
H	4.091381294	5.219862377	0.911312063
C	-4.420860321	5.961699431	-0.604660044
O	-4.138316299	4.610204333	-0.375253028
H	-3.201185228	4.484727321	-0.331363025
H	-5.496695395	6.068141439	-0.608186042
H	-4.037447289	6.301702454	-1.563657111
H	-4.017269290	6.600492476	0.176879014

Coord_2

C	-2.536504180	-0.784015058	0.256981019
C	-3.668773262	-1.580288115	0.121863006
C	-4.791233345	-1.104879079	-0.547723038
C	-4.780122343	0.201863012	-1.066671079
C	-3.683504266	0.998057074	-0.936865070
C	-2.504430181	0.518629037	-0.294711023

C	0.064244007	0.978185071	-0.119258010
C	0.520531038	-0.283905023	-0.524225039
C	1.051352075	1.880250138	0.360039024
C	1.862381134	-0.652864049	-0.463963032
C	2.381493173	1.525337111	0.402693028
C	2.795643200	0.250312020	-0.013595003
H	-1.691458121	-1.154966081	0.804464059
H	-3.677900263	-2.566818184	0.548075042
H	-5.662993410	-1.722557122	-0.653633049
H	-5.647984409	0.575766040	-1.577574113
H	-3.711005269	1.992006144	-1.337395096
C	-1.340728098	1.353281098	-0.222715014
O	-1.564551114	2.685607194	-0.489023036
H	2.143195153	-1.632638117	-0.797270059
H	3.109263224	2.221368159	0.772210055
O	4.117508299	0.022743001	0.078810008
C	4.631641335	-1.224673087	-0.293173023
H	5.695763410	-1.172445086	-0.120920007
H	4.449157323	-1.431540105	-1.342342099
H	4.211191304	-2.021800146	0.310589024
H	-0.179644013	-0.983987071	-0.933481066
O	0.754544055	3.141971225	0.781559056
H	-0.157428009	3.238647231	1.018710073
C	3.376011241	5.626803407	1.628902115
O	2.123197154	5.846855421	1.056948077
H	1.736123126	5.012318361	0.825562060
H	3.323363238	4.958723358	2.486050178
H	3.754085271	6.582506472	1.967188144
H	4.087149294	5.214131376	0.915378066
C	-4.417634319	5.964255431	-0.620108046
O	-4.135617300	4.614616332	-0.379296027
H	-3.198110232	4.483426323	-0.359480027
H	-5.493153395	6.074436436	-0.604730044
H	-4.051191292	6.291125455	-1.590453112
H	-3.996995287	6.611138475	0.145861009

Coord_3

C	-2.527988184	-0.785377054	0.251925016
C	-3.657535263	-1.583161113	0.118420010
C	-4.788925344	-1.106267079	-0.540334041
C	-4.788187343	0.210629013	-1.043682075
C	-3.696825266	1.009816075	-0.913330065
C	-2.503588181	0.527104038	-0.289176020
C	0.064567006	0.975532072	-0.122594006
C	0.522875039	-0.282006023	-0.534689038
C	1.047997076	1.875165136	0.366791024
C	1.864961133	-0.651085045	-0.470763034

C	2.378199171	1.521081108	0.414189028
C	2.795210201	0.249518016	-0.009288003
H	-1.677687119	-1.157692085	0.789979055
H	-3.660553261	-2.573383183	0.535953041
H	-5.658869405	-1.726309126	-0.645369047
H	-5.663997407	0.586415045	-1.539350111
H	-3.737071270	2.008699146	-1.297119093
C	-1.341562097	1.358137098	-0.238675016
O	-1.551643110	2.679875194	-0.537427038
H	2.148030156	-1.628256117	-0.809786059
H	3.103880221	2.215405157	0.791053057
O	4.116836296	0.022168002	0.087275008
C	4.633554332	-1.221785086	-0.292689021
H	5.697108409	-1.169775086	-0.116737009
H	4.454549321	-1.420763103	-1.343996095
H	4.212051302	-2.023998147	0.303592020
H	-0.174949015	-0.980019072	-0.951723070
O	0.747249055	3.133914227	0.793923055
H	-0.167528013	3.229769235	1.020180075
C	3.373202241	5.621886403	1.633387120
O	2.118942150	5.841123420	1.064243077
H	1.730715125	5.006212359	0.836101059
H	3.322728241	4.954755354	2.491411177
H	3.751904272	6.578051472	1.969717140
H	4.082636296	5.208544376	0.918554066
C	-4.414274318	5.965568431	-0.633052044
O	-4.132682297	4.617659334	-0.382078028
H	-3.195529228	4.480398323	-0.386405026
H	-5.489096394	6.079794436	-0.598672044
H	-4.065064293	6.280077451	-1.613993118
H	-3.976761285	6.619558479	0.117510010

Coord_4

C	-2.519744179	-0.786234057	0.246252019
C	-3.646931265	-1.585022113	0.114682008
C	-4.786863347	-1.106434077	-0.533448037
C	-4.795706343	0.220170015	-1.021566074
C	-3.709375265	1.021825075	-0.891009062
C	-2.502390182	0.535701036	-0.284839021
C	0.064912004	0.972736069	-0.126576007
C	0.525435040	-0.280342020	-0.545234037
C	1.044465077	1.870041134	0.372859025
C	1.867726137	-0.649519045	-0.477115034
C	2.374690170	1.516783109	0.425511029
C	2.794748203	0.248601016	-0.004577002
H	-1.664476119	-1.159971082	0.775080053
H	-3.644416260	-2.578628187	0.523971039

H	-5.655322409	-1.728396122	-0.637413047
H	-5.679081409	0.597808046	-1.502102107
H	-3.760457269	2.025593146	-1.258050090
C	-1.342201094	1.362621097	-0.255932020
O	-1.539730113	2.672445191	-0.587194041
H	2.153203155	-1.624150119	-0.821424058
H	3.098131224	2.209486161	0.809691061
O	4.116091294	0.021507002	0.096623008
C	4.635580334	-1.219026088	-0.290720021
H	5.698498409	-1.167164083	-0.110762011
H	4.460384321	-1.410450100	-1.344084098
H	4.212903304	-2.026091144	0.298173023
H	-0.169859012	-0.976379068	-0.970021072
O	0.739626051	3.125922227	0.805071057
H	-0.177873010	3.221134232	1.020118071
C	3.369672243	5.617439403	1.636542117
O	2.114147154	5.835604419	1.069729078
H	1.724882126	5.000229360	0.845024062
H	3.321123241	4.951577354	2.495671181
H	3.748853269	6.574205475	1.970680142
H	4.077645292	5.203185377	0.920788067
C	-4.410321317	5.965833427	-0.643392046
O	-4.129261299	4.619455330	-0.383517025
H	-3.193216232	4.475704320	-0.412062032
H	-5.484042397	6.084526439	-0.589905043
H	-4.078560292	6.268755450	-1.634201116
H	-3.956010287	6.625902478	0.091957009

Coord_5

C	-2.511817183	-0.786702056	0.239970018
C	-3.636972260	-1.586030117	0.110656006
C	-4.785074347	-1.105561077	-0.527061037
C	-4.802735346	0.230334018	-1.000330070
C	-3.721245267	1.033990077	-0.869914062
C	-2.500904178	0.544331039	-0.281707022
C	0.065219006	0.969740069	-0.131204011
C	0.528196038	-0.278965021	-0.555859038
C	1.040658075	1.864866135	0.378229026
C	1.870669135	-0.648166045	-0.483023034
C	2.370876173	1.512481110	0.436638034
C	2.794211199	0.247605019	0.000524002
H	-1.651854120	-1.161902082	0.759773056
H	-3.629462261	-2.582738185	0.512147039
H	-5.652358408	-1.729035125	-0.629751047
H	-5.693304408	0.609796043	-1.465845105
H	-3.781307271	2.042638146	-1.220249086
C	-1.342705099	1.366634097	-0.274489018

O	-1.528843111	2.663231194	-0.638270044
H	2.158741153	-1.620315119	-0.832188058
H	3.091899220	2.203681161	0.828097057
O	4.115231296	0.020850002	0.106831007
C	4.637724333	-1.216298090	-0.287284021
H	5.699933411	-1.164474084	-0.103021010
H	4.466667322	-1.400514099	-1.342628098
H	4.213787305	-2.027999145	0.294324020
H	-0.164362014	-0.973150071	-0.988367071
O	0.731534052	3.117979223	0.814984061
H	-0.188596015	3.212689229	1.018508076
C	3.365211241	5.613530403	1.638322116
O	2.108588152	5.830323421	1.073366076
H	1.718423126	4.994382359	0.852296063
H	3.318366238	4.949262357	2.498785178
H	3.744694269	6.571045472	1.970023142
H	4.071975295	5.198141376	0.922030067
C	-4.405307315	5.965232430	-0.651050045
O	-4.125099299	4.620109335	-0.383539029
H	-3.190947231	4.469393320	-0.436380033
H	-5.477498395	6.088930437	-0.578350039
H	-4.091162294	6.257334450	-1.651023121
H	-3.934173285	6.630302475	0.069306006

Coord_6

C	-2.504259178	-0.786899058	0.233089015
C	-3.627681262	-1.586348115	0.106349006
C	-4.783591343	-1.103818079	-0.521164040
C	-4.809334345	0.240985017	-0.979969070
C	-3.732525267	1.046221078	-0.850041059
C	-2.499201180	0.552899037	-0.279771021
C	0.065428004	0.966487068	-0.136471008
C	0.531140036	-0.277918023	-0.566561039
C	1.036483073	1.859629132	0.382895025
C	1.873782136	-0.647022048	-0.488496034
C	2.366672172	1.508213110	0.447555034
C	2.793557199	0.246577018	0.005996002
H	-1.639858116	-1.163595084	0.744072055
H	-3.615679258	-2.585891187	0.500486036
H	-5.649992409	-1.728424126	-0.622375046
H	-5.706734413	0.622251044	-1.430578103
H	-3.799758274	2.059779150	-1.183746085
C	-1.343134097	1.370071098	-0.294334022
O	-1.519020111	2.652141189	-0.690593048
H	2.164669156	-1.616743114	-0.842085059
H	3.085072220	2.198063156	0.846244058
O	4.114219298	0.020296001	0.117868009

C	4.639990334	-1.213492085	-0.282418019
H	5.701413409	-1.161555084	-0.093559009
H	4.473400324	-1.390853100	-1.339663097
H	4.214750301	-2.029633144	0.292019019
H	-0.158451009	-0.970407070	-1.006744074
O	0.722838051	3.110067224	0.823656059
H	-0.199825013	3.204373230	1.015353073
C	3.359612239	5.610225405	1.638683115
O	2.102044150	5.825304418	1.075126078
H	1.711141123	4.988686358	0.857895060
H	3.314281239	4.947876357	2.500714182
H	3.739194271	6.568649474	1.967695143
H	4.065428293	5.193500375	0.922230064
C	-4.398759318	5.963928431	-0.655969049
O	-4.119942297	4.619719331	-0.382072028
H	-3.188502231	4.461506319	-0.459287032
H	-5.468962396	6.093289440	-0.563955042
H	-4.102351297	6.245973449	-1.664425117
H	-3.910677281	6.632868477	0.049629005

Coord_7

C	-2.497131181	-0.786950055	0.225623018
C	-3.619089260	-1.586132116	0.101765008
C	-4.782458343	-1.101364077	-0.515749038
C	-4.815563349	0.251994021	-0.960467068
C	-3.743300268	1.058426075	-0.831366060
C	-2.497348181	0.561306039	-0.279004021
C	0.065479006	0.962924070	-0.142362010
C	0.534249037	-0.277245020	-0.577330040
C	1.031847073	1.854317134	0.386860029
C	1.877056135	-0.646075049	-0.493544035
C	2.361992171	1.504023111	0.458244034
C	2.792743203	0.245572016	0.011814999
H	-1.628535115	-1.165174085	0.727986051
H	-3.603070261	-2.588268188	0.488985036
H	-5.648251405	-1.726746126	-0.615281044
H	-5.719439414	0.635061044	-1.396288100
H	-3.815935275	2.076958148	-1.148546082
C	-1.343548099	1.372825100	-0.315437023
O	-1.510310107	2.639078189	-0.744081051
H	2.171012155	-1.613413118	-0.851129063
H	3.077541223	2.192706157	0.864108061
O	4.113016298	0.019952004	0.129690009
C	4.642384337	-1.210488089	-0.276170018
H	5.702941408	-1.158246081	-0.082441005
H	4.480579323	-1.381355099	-1.335241096
H	4.215841301	-2.030897148	0.291216019

H	-0.152121012	-0.968225071	-1.025135073
O	0.713404053	3.102167222	0.831092058
H	-0.211685013	3.196123230	1.010669071
C	3.352673244	5.607589404	1.637590116
O	2.094296149	5.820570419	1.074993080
H	1.702838120	4.983153360	0.861809061
H	3.308698239	4.947487353	2.501421179
H	3.732123267	6.567092470	1.963656140
H	4.057805294	5.189352371	0.921343068
C	-4.390196314	5.962068431	-0.658116048
O	-4.113536294	4.618373332	-0.379054029
H	-3.185667227	4.452074322	-0.480715032
H	-5.457920393	6.097872437	-0.546697038
H	-4.111597293	6.234804448	-1.674398119
H	-3.884938279	6.633690480	0.032965001

Coord_8

C	-2.490498177	-0.786984054	0.217590017
C	-3.611243260	-1.585535114	0.096905007
C	-4.781726343	-1.098346079	-0.510806035
C	-4.821485345	0.263246017	-0.941798065
C	-3.753654272	1.070522077	-0.813847060
C	-2.495415181	0.569451040	-0.279370021
C	0.065315004	0.958998067	-0.148853009
C	0.537504038	-0.276982019	-0.588156043
C	1.026663073	1.848921135	0.390133027
C	1.880484134	-0.645306048	-0.498180035
C	2.356757168	1.499953108	0.468690035
C	2.791730199	0.244647019	0.017951999
H	-1.617942119	-1.166773084	0.711529051
H	-3.591655256	-2.590043186	0.477629035
H	-5.647176408	-1.724162122	-0.608467046
H	-5.731487414	0.648131045	-1.362946097
H	-3.829954276	2.094114149	-1.114626080
C	-1.344010097	1.374788099	-0.337757026
O	-1.502768109	2.623943191	-0.798642057
H	2.177793159	-1.610299117	-0.859343063
H	3.069201220	2.187683159	0.881661061
O	4.111588297	0.019927000	0.142246009
C	4.644911333	-1.207158087	-0.268607022
H	5.704520409	-1.154375086	-0.069752007
H	4.488196321	-1.371893098	-1.329428094
H	4.217112305	-2.031687146	0.291857022
H	-0.145366012	-0.966669068	-1.043518077
O	0.703105052	3.094256223	0.837309059
H	-0.224294015	3.187870229	1.004489075
C	3.344192242	5.605684403	1.635016118

O	2.085125152	5.816138417	1.072966077
H	1.693321121	4.977792361	0.864043062
H	3.301454236	4.948153355	2.500876179
H	3.723252266	6.566447472	1.957874143
H	4.048908289	5.185787373	0.919330067
C	-4.379132313	5.959779427	-0.657481046
O	-4.105628296	4.616145332	-0.374427025
H	-3.182234227	4.441116321	-0.500600037
H	-5.443847390	6.102931441	-0.526580036
H	-4.118365296	6.223939450	-1.680954122
H	-3.856372275	6.632830477	0.019324003

Coord_9

C	-2.484435177	-0.787134055	0.209015017
C	-3.604198260	-1.584705115	0.091769008
C	-4.781457346	-1.094898076	-0.506323036
C	-4.827168349	0.274641018	-0.923925067
C	-3.763670269	1.082424078	-0.797429055
C	-2.493472180	0.577226040	-0.280815019
C	0.064879004	0.954659067	-0.155911011
C	0.540886036	-0.277161019	-0.599026042
C	1.020844076	1.843429133	0.392728027
C	1.884058134	-0.644691044	-0.502424037
C	2.350890170	1.496051109	0.478878036
C	2.790480203	0.243866017	0.024377000
H	-1.608145116	-1.168535086	0.694715048
H	-3.581473256	-2.591385185	0.466399031
H	-5.646817409	-1.720819124	-0.601934046
H	-5.742947414	0.661385046	-1.330513098
H	-3.841921275	2.111180152	-1.081941076
C	-1.344582096	1.375851100	-0.361235028
O	-1.496459109	2.606634189	-0.854167059
H	2.185036156	-1.607364114	-0.866757064
H	3.059953218	2.183071157	0.898879065
O	4.109903297	0.020342002	0.155473011
C	4.647579333	-1.203362087	-0.259810016
H	5.706155408	-1.149762084	-0.055596002
H	4.496242324	-1.362325097	-1.322307094
H	4.218623302	-2.031893144	0.293866023
H	-0.138184007	-0.965799069	-1.061866076
O	0.691817051	3.086309224	0.842336058
H	-0.237768016	3.179538227	0.996862070
C	3.333974242	5.604570405	1.630944115
O	2.074313151	5.812026419	1.069059076
H	1.682395119	4.972613356	0.864616061
H	3.292395235	4.949930358	2.499056180
H	3.712359269	6.566781473	1.950327139

H	4.038541289	5.182897372	0.916154067
C	-4.365075312	5.957166429	-0.654080045
O	-4.095965297	4.613099334	-0.368142024
H	-3.178001227	4.428641317	-0.518878036
H	-5.426209388	6.108701441	-0.503641039
H	-4.122109299	6.213460449	-1.684132122
H	-3.824386273	6.630323478	0.008679999

Coord_10

C	-2.469552178	-0.786661055	0.212133014
C	-3.585748257	-1.587487116	0.103219007
C	-4.770590342	-1.103014079	-0.489884034
C	-4.825860350	0.271153021	-0.904117063
C	-3.769465273	1.083573080	-0.784134054
C	-2.486341178	0.581915043	-0.280710020
C	0.068000007	0.956758070	-0.161327013
C	0.552811040	-0.272376018	-0.598701043
C	1.014688072	1.851853132	0.391392030
C	1.897346135	-0.633466046	-0.491354035
C	2.345777169	1.511574110	0.489077033
C	2.795050199	0.260839017	0.040509005
H	-1.588874116	-1.163384085	0.693201050
H	-3.557207257	-2.593452188	0.479232034
H	-5.633900404	-1.732291126	-0.579618043
H	-5.748039412	0.653934045	-1.299760095
H	-3.851235276	2.115423153	-1.059855075
C	-1.342683096	1.376446102	-0.387819030
O	-1.492456106	2.583363186	-0.921179065
H	2.205914156	-1.595344112	-0.851445061
H	3.048457218	2.203529160	0.911781068
O	4.114647296	0.044318002	0.181438014
C	4.661612336	-1.177021083	-0.228686017
H	5.718691411	-1.117220080	-0.018394000
H	4.517371323	-1.338533097	-1.291800094
H	4.233993303	-2.007052146	0.323815026
H	-0.119393008	-0.965811071	-1.064656078
O	0.675202049	3.094318221	0.833918060
H	-0.256870019	3.184900227	0.974107072
C	3.308343240	5.634694408	1.597541113
O	2.047976148	5.830402422	1.032983074
H	1.659228120	4.987066361	0.838821062
H	3.269335236	4.989260357	2.472645176
H	3.682194266	6.602018475	1.906717139
H	4.015083290	5.208555372	0.887559064
C	-4.360151313	5.942669428	-0.684713047
O	-4.092620293	4.600604332	-0.387243026
H	-3.180290231	4.407835316	-0.560427039

H	-5.417771392	6.101358440	-0.516746039
H	-4.134837298	6.185255445	-1.722292126
H	-3.803863276	6.620969477	-0.040054003

LIIC path connecting S₁/T₁-ENOL and T1-PP-ENOL

Coord_1

C	-2.469552178	-0.786661055	0.212133014
C	-3.585748257	-1.587487116	0.103219007
C	-4.770590342	-1.103014079	-0.489884034
C	-4.825860350	0.271153021	-0.904117063
C	-3.769465273	1.083573080	-0.784134054
C	-2.486341178	0.581915043	-0.280710020
C	0.068000007	0.956758070	-0.161327013
C	0.552811040	-0.272376018	-0.598701043
C	1.014688072	1.851853132	0.391392030
C	1.897346135	-0.633466046	-0.491354035
C	2.345777169	1.511574110	0.489077033
C	2.795050199	0.260839017	0.040509005
H	-1.588874116	-1.163384085	0.693201050
H	-3.557207257	-2.593452188	0.479232034
H	-5.633900404	-1.732291126	-0.579618043
H	-5.748039412	0.653934045	-1.299760095
H	-3.851235276	2.115423153	-1.059855075
C	-1.342683096	1.376446102	-0.387819030
O	-1.492456106	2.583363186	-0.921179065
H	2.205914156	-1.595344112	-0.851445061
H	3.048457218	2.203529160	0.911781068
O	4.114647296	0.044318002	0.181438014
C	4.661612336	-1.177021083	-0.228686017
H	5.718691411	-1.117220080	-0.018394000
H	4.517371323	-1.338533097	-1.291800094
H	4.233993303	-2.007052146	0.323815026
H	-0.119393008	-0.965811071	-1.064656078
O	0.675202049	3.094318221	0.833918060
H	-0.256870019	3.184900227	0.974107072
C	3.308343240	5.634694408	1.597541113
O	2.047976148	5.830402422	1.032983074
H	1.659228120	4.987066361	0.838821062
H	3.269335236	4.989260357	2.472645176
H	3.682194266	6.602018475	1.906717139
H	4.015083290	5.208555372	0.887559064
C	-4.360151313	5.942669428	-0.684713047
O	-4.092620293	4.600604332	-0.387243026
H	-3.180290231	4.407835316	-0.560427039
H	-5.417771392	6.101358440	-0.516746039
H	-4.134837298	6.185255445	-1.722292126
H	-3.803863276	6.620969477	-0.040054003

Coord_2

C	-2.474542176	-0.775232054	0.234585015
C	-3.586172260	-1.584847114	0.111524010
C	-4.763907341	-1.110875081	-0.502161036
C	-4.822588346	0.254654020	-0.928767065
C	-3.764207273	1.071438077	-0.791184055
C	-2.497664179	0.584839044	-0.260946017
C	0.058855004	0.982155070	-0.145787009
C	0.536215037	-0.259959017	-0.594423042
C	1.017764074	1.879552137	0.373285029
C	1.887101136	-0.632575044	-0.483629037
C	2.353474169	1.534762112	0.448161032
C	2.791125201	0.263767019	0.018728001
H	-1.597313117	-1.146192085	0.726981053
H	-3.557653258	-2.589490185	0.491035037
H	-5.620994406	-1.747415128	-0.602363045
H	-5.739223414	0.628404048	-1.345493095
H	-3.852972280	2.094870153	-1.074723077
C	-1.354934099	1.404579101	-0.334377023
O	-1.504935111	2.636064191	-0.783510059
H	2.184518155	-1.605238113	-0.823707061
H	3.068015223	2.231639161	0.841247059
O	4.110610293	0.048667003	0.156665010
C	4.652415336	-1.181447085	-0.234344017
H	5.711148413	-1.119973082	-0.033277004
H	4.498923326	-1.362300098	-1.292986092
H	4.226915303	-1.999613146	0.337011024
H	-0.133965009	-0.916036066	-1.114743081
O	0.700463050	3.128011223	0.812545056
H	-0.232387014	3.234161231	0.940509069
C	3.359896243	5.614553403	1.622989115
O	2.113293152	5.836351422	1.038080077
H	1.711137122	5.001134359	0.836418062
H	3.293800238	4.966734356	2.494662178
H	3.747025269	6.573330475	1.942207141
H	4.070375291	5.177537373	0.923329065
C	-4.396663315	5.915737423	-0.714743052
O	-4.168776298	4.575843330	-0.377952028
H	-3.245157233	4.377159313	-0.459075033
H	-5.463455391	6.085314437	-0.644734045
H	-4.076836291	6.143190441	-1.730553122
H	-3.894755279	6.598243473	-0.031309005

Coord_3

C	-2.482077179	-0.765754056	0.256250019
C	-3.589364258	-1.583340113	0.119478010

C	-4.758184342	-1.119395083	-0.516117038
C	-4.817517346	0.236653019	-0.957328068
C	-3.757753268	1.057726074	-0.803185059
C	-2.509359182	0.585105040	-0.244193017
C	0.047965002	1.005750072	-0.131145008
C	0.518467035	-0.249602018	-0.589623044
C	1.017546074	1.906465139	0.353062023
C	1.875957134	-0.632304047	-0.474199035
C	2.357631168	1.557840114	0.405550029
C	2.785021200	0.266863018	-0.002206002
H	-1.609295114	-1.130849082	0.761426053
H	-3.562172257	-2.586044188	0.504155034
H	-5.609599404	-1.762231128	-0.626359047
H	-5.727108414	0.601815045	-1.396608099
H	-3.849769276	2.073446147	-1.097293080
C	-1.368265101	1.428843105	-0.282800021
O	-1.522008110	2.677706192	-0.647769046
H	2.163299158	-1.615309118	-0.792655056
H	3.082787222	2.260025160	0.767891053
O	4.104554294	0.054594005	0.133311010
C	4.642585334	-1.183901086	-0.236625015
H	5.702795408	-1.119688078	-0.044629005
H	4.480305320	-1.385508098	-1.290142092
H	4.219973302	-1.989475142	0.354276024
H	-0.145321010	-0.867950063	-1.162225086
O	0.720296053	3.160729225	0.786643058
H	-0.213172017	3.281200236	0.901576065
C	3.397500245	5.601343403	1.641609116
O	2.165304158	5.844747422	1.035343072
H	1.752259126	5.016494363	0.827208061
H	3.305378239	4.953038354	2.510519180
H	3.794884271	6.552913473	1.969590143
H	4.112982298	5.153906370	0.953635067
C	-4.409625316	5.889241423	-0.730317050
O	-4.231658303	4.548503329	-0.368972028
H	-3.307165239	4.337834310	-0.363364024
H	-5.475556394	6.075723438	-0.751836054
H	-4.001532289	6.105809440	-1.716297124
H	-3.957021285	6.568533473	-0.010463999

Coord_4

C	-2.491840181	-0.757239054	0.276914020
C	-3.595043261	-1.581992113	0.127011007
C	-4.752939344	-1.127829084	-0.532093037
C	-4.809885346	0.217692016	-0.990481070
C	-3.749308272	1.043021074	-0.821057058
C	-2.520774180	0.583501040	-0.231136018

C	0.035951001	1.027755072	-0.117738006
C	0.499849034	-0.241343016	-0.584399043
C	1.014866071	1.932456140	0.330438023
C	1.864052133	-0.633120043	-0.462762033
C	2.358958170	1.580118111	0.361303027
C	2.777116202	0.269308018	-0.021900000
H	-1.624673116	-1.116190079	0.796592056
H	-3.570675257	-2.581968185	0.518888038
H	-5.599286401	-1.776004130	-0.651850045
H	-5.710764410	0.574558040	-1.453976104
H	-3.840671274	2.051680150	-1.128725081
C	-1.381949100	1.449943106	-0.233796017
O	-1.542840109	2.709204197	-0.515048037
H	2.142127152	-1.626094116	-0.757804057
H	3.093662222	2.287690166	0.691823052
O	4.096749294	0.060827004	0.112073010
C	4.632042335	-1.185813083	-0.234525017
H	5.693535409	-1.118173081	-0.051231004
H	4.461640323	-1.409672104	-1.282197093
H	4.212625306	-1.977759142	0.376578025
H	-0.153247011	-0.821627061	-1.207438086
O	0.735755050	3.192510230	0.755752055
H	-0.198200015	3.326220239	0.856602063
C	3.422787245	5.595068404	1.653368117
O	2.205677159	5.855746424	1.024421076
H	1.784101129	5.033238362	0.810810059
H	3.305442238	4.948096357	2.520192181
H	3.827571274	6.540866472	1.988839145
H	4.144617298	5.137538367	0.978692070
C	-4.403622319	5.863147423	-0.730474052
O	-4.283027306	4.518815326	-0.360352027
H	-3.366689244	4.290127309	-0.274848022
H	-5.460103392	6.072822435	-0.835715061
H	-3.914340283	6.072525435	-1.680245120
H	-3.995279287	6.531847471	0.024664999

Coord_5

C	-2.503496178	-0.748478054	0.296414022
C	-3.602919260	-1.579595115	0.134089012
C	-4.747626341	-1.135198083	-0.550392039
C	-4.798807343	0.198503012	-1.028814072
C	-3.737944270	1.028092074	-0.845625059
C	-2.531192183	0.581008044	-0.222358015
C	0.023463000	1.048626077	-0.105811007
C	0.480569032	-0.234973019	-0.578831040
C	1.010691075	1.957503142	0.305236020
C	1.851402135	-0.635335047	-0.449069032

C	2.358291169	1.600917116	0.315519024
C	2.767768201	0.270335018	-0.040007001
H	-1.643318121	-1.100812077	0.832590058
H	-3.583105260	-2.575857187	0.535539039
H	-5.589572400	-1.787747129	-0.679068049
H	-5.689090410	0.547202037	-1.518372112
H	-3.824519276	2.030242148	-1.170062085
C	-1.395254098	1.468843106	-0.187924012
O	-1.566803112	2.731667195	-0.386163028
H	2.120632152	-1.637950120	-0.718782050
H	3.101743224	2.313541168	0.613213046
O	4.087444294	0.066065007	0.093531005
C	4.620558331	-1.188628083	-0.227240014
H	5.683145411	-1.117326079	-0.052107004
H	4.442818319	-1.436230102	-1.268275091
H	4.204160300	-1.965600141	0.404652031
H	-0.157516011	-0.776845055	-1.250657092
O	0.748138052	3.223452234	0.719616049
H	-0.186157015	3.369524242	0.805133056
C	3.437671249	5.595548404	1.658419119
O	2.236410160	5.869393424	1.005242073
H	1.808465132	5.051407362	0.787104056
H	3.295638239	4.951629356	2.523786183
H	3.847203279	6.537028471	2.000140144
H	4.167194301	5.128148371	0.998851072
C	-4.383688318	5.836771419	-0.714649054
O	-4.324764309	4.486647324	-0.352318026
H	-3.424082247	4.234373305	-0.195141016
H	-5.423653388	6.075638436	-0.894515062
H	-3.820841277	6.042579437	-1.623413118
H	-4.015088291	6.487387465	0.075692006

Coord_6

C	-2.516652181	-0.738063052	0.314644024
C	-3.612633261	-1.574741115	0.140703008
C	-4.741588344	-1.140347084	-0.571255043
C	-4.783260343	0.179954016	-1.072767080
C	-3.722593266	1.013849072	-0.877557064
C	-2.539808183	0.578780044	-0.218293013
C	0.011168000	1.069101077	-0.095479007
C	0.460722033	-0.229998017	-0.572963041
C	1.006128074	1.981723140	0.277430021
C	1.837863130	-0.639083046	-0.432936031
C	2.356581169	1.619591115	0.268360018
C	2.757287200	0.269247019	-0.056235005
H	-1.665072121	-1.083085078	0.869562063
H	-3.599354261	-2.566087184	0.554386041

H	-5.579863400	-1.796291129	-0.708223054
H	-5.660815406	0.520412036	-1.590403116
H	-3.799968272	2.009884143	-1.222154087
C	-1.407457100	1.486768107	-0.145539010
O	-1.593536115	2.746339200	-0.261651019
H	2.098146151	-1.651033117	-0.675360051
H	3.108349224	2.336415166	0.532305036
O	4.076833296	0.068979006	0.078119008
C	4.607715332	-1.193810083	-0.214226016
H	5.671238410	-1.119156080	-0.046595004
H	4.423412320	-1.466542105	-1.247759090
H	4.193669303	-1.954162139	0.438931033
H	-0.157943010	-0.733050055	-1.292062095
O	0.759012057	3.253739234	0.678235050
H	-0.175416014	3.411552246	0.747036056
C	3.444416248	5.602420401	1.657109120
O	2.259889162	5.885640425	0.978056068
H	1.827497130	5.071014363	0.756265056
H	3.277971234	4.963156355	2.521540180
H	3.856307276	6.540986468	2.003903144
H	4.182895302	5.125289369	1.014593074
C	-4.355363312	5.808857420	-0.682748048
O	-4.358931316	4.451464319	-0.345284027
H	-3.479703248	4.170928303	-0.125902010
H	-5.373397387	6.082097436	-0.926931069
H	-3.726876268	6.015134431	-1.547135113
H	-4.022902292	6.433626464	0.143454010

Coord_7

C	-2.530775181	-0.724381052	0.331564022
C	-3.623640259	-1.565860113	0.146876008
C	-4.733971340	-1.142016082	-0.594828042
C	-4.762045341	0.162979010	-1.122559081
C	-3.702034264	1.001301073	-0.917298064
C	-2.545709182	0.578152042	-0.219179015
C	-0.000267002	1.090265077	-0.086678006
C	0.440229031	-0.225564014	-0.566791041
C	1.002427072	2.005426143	0.247188017
C	1.823048130	-0.644294044	-0.414263028
C	2.354881172	1.635547116	0.220064016
C	2.745872196	0.265428021	-0.070370006
H	-1.689644123	-1.061114078	0.907670065
H	-3.619107263	-2.550838185	0.575661041
H	-5.569337403	-1.800380129	-0.739477056
H	-5.624465406	0.494853035	-1.670418118
H	-3.765511271	1.991376143	-1.285576091
C	-1.417861101	1.505231106	-0.106726007

O	-1.622994116	2.754576199	-0.141761013
H	2.073605149	-1.665278119	-0.627494043
H	3.115011227	2.355083169	0.449439033
O	4.065001295	0.068193003	0.066080004
C	4.592808329	-1.202881086	-0.195274014
H	5.657166406	-1.125837081	-0.034437003
H	4.402556318	-1.501899110	-1.220369087
H	4.179956299	-1.944686141	0.479476033
H	-0.154482010	-0.689276047	-1.331705097
O	0.770256058	3.283695238	0.631931046
H	-0.163989013	3.452961249	0.682591052
C	3.445766248	5.615136403	1.650024119
O	2.278993164	5.904379427	0.943495068
H	1.843770134	5.092084365	0.718833052
H	3.254941233	4.981987361	2.513881181
H	3.857978275	6.552054470	2.000801144
H	4.194269300	5.128330371	1.026539076
C	-4.324802310	5.777592416	-0.635270048
O	-4.387848318	4.412276320	-0.339902025
H	-3.533918256	4.100140294	-0.068871006
H	-5.317362385	6.089035437	-0.932343065
H	-3.638735262	5.989331431	-1.453134103
H	-4.026069290	6.368389456	0.227788014

Coord_8

C	-2.545045181	-0.705577051	0.347224023
C	-3.635003261	-1.551256112	0.152707012
C	-4.723544341	-1.138949082	-0.621091046
C	-4.733714340	0.148466011	-1.178098086
C	-3.674873263	0.991514072	-0.964987067
C	-2.547823181	0.580682044	-0.224998017
C	-0.010204003	1.113699083	-0.079100008
C	0.418718028	-0.220313015	-0.560249039
C	1.000994071	2.029216147	0.214939014
C	1.806193131	-0.650630048	-0.393077030
C	2.354310168	1.648292117	0.170971015
C	2.733512198	0.258361018	-0.082305007
H	-1.716435123	-1.032637076	0.947095066
H	-3.641550263	-2.528142180	0.599578043
H	-5.556722400	-1.798842129	-0.772869056
H	-5.578321399	0.471026035	-1.758400128
H	-3.719551270	1.975455141	-1.360541097
C	-1.425820101	1.526121108	-0.071218008
O	-1.655535119	2.757872200	-0.026465001
H	2.045351148	-1.680343123	-0.575404041
H	3.123464225	2.368259169	0.365076024
O	4.051803291	0.062232006	0.057410006

C	4.574672329	-1.217497089	-0.170621012
H	5.639850404	-1.139846080	-0.015910000
H	4.378710316	-1.543573109	-1.186292083
H	4.161373298	-1.938569138	0.525849036
H	-0.147363010	-0.643969045	-1.369492099
O	0.784142055	3.313887240	0.581448044
H	-0.149441010	3.494780254	0.612620045
C	3.445174247	5.632943408	1.638073117
O	2.297302168	5.925486424	0.902695063
H	1.860446134	5.114714370	0.675823049
H	3.229774230	5.007195359	2.501510181
H	3.856153275	6.569240475	1.991873141
H	4.204433303	5.136405367	1.035508075
C	-4.299001310	5.740592412	-0.573512042
O	-4.414199318	4.367549317	-0.337188023
H	-3.587120260	4.022347291	-0.025926002
H	-5.264755377	6.092083439	-0.911066065
H	-3.563495258	5.964306428	-1.343658099
H	-4.032893290	6.288916452	0.327244026

Coord_9

C	-2.558084182	-0.679437049	0.361838025
C	-3.644993264	-1.529152109	0.158468012
C	-4.708367337	-1.130099079	-0.649744046
C	-4.696409339	0.137060008	-1.238872087
C	-3.639496261	0.985567072	-1.020387073
C	-2.544825181	0.588278045	-0.235406018
C	-0.018071001	1.141777085	-0.072099003
C	0.395325028	-0.212092014	-0.553203039
C	1.003421073	2.054180148	0.181472013
C	1.785889129	-0.657362045	-0.369588027
C	2.356009171	1.657489117	0.121552009
C	2.719784197	0.247660017	-0.092089007
H	-1.744215124	-0.994776074	0.988094074
H	-3.664823266	-2.495916180	0.626439043
H	-5.539860399	-1.790911127	-0.808189060
H	-5.520294399	0.448947030	-1.853846135
H	-3.660537264	1.962752141	-1.446858104
C	-1.430781101	1.551926114	-0.038282005
O	-1.692102119	2.757986201	0.084545009
H	2.010771145	-1.695504120	-0.519690038
H	3.135646224	2.374582171	0.279834020
O	4.036655291	0.049416006	0.051753006
C	4.551338327	-1.239604088	-0.141131011
H	5.617436403	-1.164226085	0.007966001
H	4.349234312	-1.592906113	-1.146384081
H	4.135467299	-1.937520139	0.576935041

H	-0.137359009	-0.594636041	-1.405160100
O	0.803491056	3.345329243	0.528110036
H	-0.128712010	3.538711253	0.538686040
C	3.447236250	5.654808409	1.622673117
O	2.319503170	5.948884430	0.857507062
H	1.881604133	5.139189369	0.628919043
H	3.206841233	5.037546363	2.485586179
H	3.856153275	6.591125473	1.978733140
H	4.217448301	5.148276369	1.042634076
C	-4.286222309	5.694782410	-0.499896036
O	-4.441242318	4.315037312	-0.338720023
H	-3.639787261	3.937917283	0.000821003
H	-5.226563375	6.085340435	-0.864773062
H	-3.509658252	5.939166428	-1.221766089
H	-4.052885289	6.191906446	0.438694030

Coord_10

C	-2.578486188	-0.735807053	0.390876029
C	-3.664826262	-1.583054114	0.168210011
C	-4.704628340	-1.179017087	-0.660382049
C	-4.668483337	0.078489004	-1.256158091
C	-3.611395261	0.926666067	-1.023365076
C	-2.547440184	0.524556039	-0.206564016
C	-0.033370002	1.089458076	-0.026326002
C	0.351649024	-0.275816019	-0.541001037
C	1.005283074	1.986073141	0.199334016
C	1.743178127	-0.749114056	-0.360360028
C	2.353191170	1.565669112	0.104642007
C	2.690949196	0.139226010	-0.102580010
H	-1.777685130	-1.052686078	1.033468075
H	-3.698261268	-2.548139185	0.638848048
H	-5.537050399	-1.835154134	-0.834141060
H	-5.472475392	0.393670026	-1.895383136
H	-3.605607258	1.906053138	-1.462526105
C	-1.440857101	1.499104107	0.050867004
O	-1.738941127	2.665981190	0.277831021
H	1.945814140	-1.792959128	-0.502702035
H	3.148413228	2.270417164	0.237104015
O	4.006073291	-0.072519006	0.031629004
C	4.503075325	-1.369144101	-0.158121009
H	5.571480402	-1.306192096	-0.020529003
H	4.285357311	-1.725813123	-1.158858085
H	4.085593296	-2.056856149	0.568679039
H	-0.150002012	-0.594185044	-1.437738104
O	0.831180060	3.276348236	0.555861038
H	-0.098118008	3.486479251	0.556524039
C	3.471170249	5.543593401	1.720880122

O	2.359988171	5.859396424	0.940463068
H	1.917111138	5.057327363	0.695296052
H	3.209706231	4.916922356	2.570750182
H	3.883127281	6.470683466	2.096949152
H	4.246486305	5.037338364	1.147316083
C	-4.298659308	5.563532403	-0.249057018
O	-4.477743324	4.178010303	-0.207614015
H	-3.695704267	3.764223270	0.133435012
H	-5.220090378	5.998552430	-0.611517044
H	-3.494331252	5.853720421	-0.921711068
H	-4.091298292	5.978250428	0.734430054

LIIC path connecting T2-NP-ENOL and T₂/T₁-ENOL and
Coord_1

C	-2.681157195	-0.782588057	0.402199030
C	-3.810428276	-1.561298113	0.145473011
C	-4.796031343	-1.096028076	-0.716977053
C	-4.653830335	0.150588012	-1.317709094
C	-3.540105254	0.918656065	-1.073146076
C	-2.525517180	0.459548032	-0.218119014
C	0.000629001	1.019296073	-0.006519998
C	0.435151030	-0.320303025	-0.350518024
C	1.077250079	1.966075141	0.239616020
C	1.733753126	-0.682882052	-0.409203030
C	2.394200174	1.579338115	0.179370010
C	2.755256197	0.258267020	-0.129515010
H	-1.938832139	-1.133594083	1.095291081
H	-3.922086284	-2.515419182	0.627458043
H	-5.668583406	-1.691918124	-0.908322064
H	-5.416328389	0.518859039	-1.979137141
H	-3.453206248	1.884642134	-1.535648109
C	-1.362595099	1.338241097	0.054113004
O	-1.716114124	2.603779188	0.414091029
H	1.978754144	-1.690383124	-0.685161049
H	3.164370229	2.303532166	0.363089027
O	4.073254295	-0.008716999	-0.146101012
C	4.525313327	-1.297450093	-0.454264034
H	5.601710404	-1.258297089	-0.388351028
H	4.241243306	-1.589323113	-1.459809103
H	4.153067300	-2.029785145	0.254147021
H	-0.311593021	-1.045286074	-0.599393043
O	0.851550061	3.273152233	0.538261037
H	-0.056050004	3.509995253	0.403730030
C	3.476136249	5.635564407	1.706892121
O	2.323109168	5.869112420	0.958807071
H	1.929676139	5.037074363	0.728756052
H	3.283376234	4.998744361	2.567500182

H	3.834549275	6.591427474	2.065821147
H	4.266514309	5.178814373	1.113109082
C	-4.217479306	5.544240400	-0.278316022
O	-4.529164324	4.182285298	-0.196332014
H	-3.921287284	3.752046272	0.388764030
H	-4.956558356	6.005292433	-0.918524067
H	-3.234045230	5.713035411	-0.711356053
H	-4.255782308	6.030295434	0.693171051

Coord_2

C	-2.681417195	-0.782671059	0.402328028
C	-3.810741273	-1.561255112	0.145550012
C	-4.796392347	-1.095854078	-0.716816051
C	-4.654138337	0.150768012	-1.317492094
C	-3.540288254	0.918701066	-1.073007077
C	-2.525646183	0.459435032	-0.218078014
C	0.001259003	1.018623071	-0.006507002
C	0.435694029	-0.320562025	-0.350521025
C	1.077335075	1.965373140	0.239606018
C	1.734575123	-0.683079048	-0.409268029
C	2.394495174	1.578904115	0.179344012
C	2.755740198	0.258067018	-0.129605007
H	-1.939132140	-1.133707084	1.095438081
H	-3.922419284	-2.515414181	0.627444046
H	-5.669001408	-1.691664119	-0.908125067
H	-5.416659390	0.519151039	-1.978823143
H	-3.453306246	1.884673133	-1.535509110
C	-1.362297098	1.337405097	0.054161006
O	-1.716158125	2.602934187	0.414484028
H	1.979691142	-1.690540120	-0.685265048
H	3.164519230	2.303247167	0.363127027
O	4.073821293	-0.008660002	-0.146245012
C	4.526007327	-1.297319095	-0.454474032
H	5.602406404	-1.258048090	-0.388602027
H	4.241858306	-1.589182113	-1.460006105
H	4.153798301	-2.029710145	0.253910018
H	-0.310957024	-1.045642073	-0.599443045
O	0.851493063	3.272507235	0.538362041
H	-0.055915006	3.509742254	0.403595032
C	3.475783251	5.635482406	1.706960125
O	2.322717165	5.868662424	0.958813067
H	1.929590137	5.036487362	0.728722052
H	3.283149238	4.998617359	2.567563186
H	3.833853275	6.591477476	2.065880151
H	4.266315306	5.178970374	1.113203080
C	-4.217803305	5.545124401	-0.278678022
O	-4.529890324	4.183265303	-0.196366014

H	-3.922810283	3.753264268	0.389713030
H	-4.956241358	6.006008431	-0.919723066
H	-3.233979231	5.713466410	-0.710972050
H	-4.256828307	6.031603433	0.692557052

Coord_3

C	-2.681675196	-0.782753055	0.402457031
C	-3.811053276	-1.561212111	0.145627012
C	-4.796750346	-1.095678078	-0.716655054
C	-4.654443334	0.150949012	-1.317275094
C	-3.540469253	0.918746067	-1.072867078
C	-2.525773180	0.459323032	-0.218037018
C	0.001887999	1.017950074	-0.006495000
C	0.436236034	-0.320821026	-0.350524025
C	1.077420077	1.964670144	0.239596017
C	1.735397126	-0.683275050	-0.409334028
C	2.394790175	1.578470116	0.179319013
C	2.756222199	0.257866020	-0.129695009
H	-1.939431141	-1.133819079	1.095583081
H	-3.922751280	-2.515407180	0.627428044
H	-5.669416410	-1.691408119	-0.907928065
H	-5.416988390	0.519444039	-1.978509140
H	-3.453404250	1.884704138	-1.535369110
C	-1.361998097	1.336569098	0.054209002
O	-1.716202121	2.602088186	0.414877032
H	1.980628140	-1.690697122	-0.685369047
H	3.164668230	2.302961168	0.363166027
O	4.074387296	-0.008601998	-0.146389012
C	4.526700327	-1.297189092	-0.454682031
H	5.603099404	-1.257800091	-0.388852026
H	4.242471305	-1.589041114	-1.460202107
H	4.154528301	-2.029635145	0.253674016
H	-0.310320022	-1.045997077	-0.599494041
O	0.851435060	3.271860237	0.538464040
H	-0.055780002	3.509488254	0.403459028
C	3.475430253	5.635398404	1.707027124
O	2.322326166	5.868209421	0.958818067
H	1.929504141	5.035898362	0.728688052
H	3.282921237	4.998488361	2.567626185
H	3.833156274	6.591524472	2.065938148
H	4.266116309	5.179124375	1.113296082
C	-4.218127304	5.546006402	-0.279039021
O	-4.530613328	4.184242302	-0.196399014
H	-3.924331281	3.754482270	0.390663030
H	-4.955925355	6.006719434	-0.920921065
H	-3.233916233	5.713896409	-0.710587052
H	-4.257874305	6.032909432	0.691943048

Coord_4

C	-2.681933191	-0.782835056	0.402585028
C	-3.811364274	-1.561168110	0.145703013
C	-4.797109345	-1.095502079	-0.716495052
C	-4.654748336	0.151130011	-1.317058095
C	-3.540651253	0.918792069	-1.072728079
C	-2.525901183	0.459211031	-0.217997018
C	0.002518000	1.017277072	-0.006481998
C	0.436778033	-0.321079021	-0.350527026
C	1.077506079	1.963967143	0.239586016
C	1.736218124	-0.683472047	-0.409398032
C	2.395084175	1.578036111	0.179294015
C	2.756705200	0.257665018	-0.129784012
H	-1.939729142	-1.133931079	1.095728080
H	-3.923082280	-2.515400179	0.627412047
H	-5.669831407	-1.691152124	-0.907731063
H	-5.417316390	0.519738039	-1.978195142
H	-3.453501248	1.884736137	-1.535230111
C	-1.361699096	1.335733098	0.054256004
O	-1.716246122	2.601242185	0.415269031
H	1.981564143	-1.690853123	-0.685473052
H	3.164816225	2.302675164	0.363205028
O	4.074952293	-0.008545001	-0.146531011
C	4.527392327	-1.297058095	-0.454890034
H	5.603792404	-1.257552092	-0.389100031
H	4.243085304	-1.588901115	-1.460397103
H	4.155257301	-2.029559144	0.253438018
H	-0.309684025	-1.046351075	-0.599544043
O	0.851378062	3.271214233	0.538565039
H	-0.055645004	3.509234254	0.403323029
C	3.475078249	5.635314408	1.707094123
O	2.321935168	5.867756424	0.958823068
H	1.929418139	5.035308361	0.728654053
H	3.282695236	4.998360359	2.567687183
H	3.832460274	6.591571474	2.065994146
H	4.265917307	5.179278371	1.113389080
C	-4.218453304	5.546886397	-0.279400021
O	-4.531335327	4.185218300	-0.196429013
H	-3.925850285	3.755701273	0.391614030
H	-4.955612357	6.007426430	-0.922116069
H	-3.233855235	5.714327413	-0.710202049
H	-4.258922309	6.034215436	0.691328049

Coord_5

C	-2.682190191	-0.782916057	0.402713031
C	-3.811675276	-1.561124114	0.145778008

C	-4.797467344	-1.095326080	-0.716336050
C	-4.655053337	0.151312011	-1.316842095
C	-3.540831253	0.918839065	-1.072589075
C	-2.526028180	0.459099031	-0.217957017
C	0.003147001	1.016604075	-0.006470002
C	0.437320032	-0.321337021	-0.350531026
C	1.077590075	1.963264141	0.239576019
C	1.737039126	-0.683668049	-0.409463030
C	2.395379170	1.577601111	0.179269012
C	2.757187196	0.257465020	-0.129873009
H	-1.940027137	-1.134043080	1.095872080
H	-3.923412280	-2.515393183	0.627395044
H	-5.670246409	-1.690896124	-0.907535066
H	-5.417644390	0.520032040	-1.977882144
H	-3.453599246	1.884768137	-1.535090112
C	-1.361400100	1.334898094	0.054302005
O	-1.716290123	2.600396190	0.415660029
H	1.982500142	-1.691010120	-0.685576051
H	3.164963225	2.302388164	0.363244028
O	4.075518296	-0.008488003	-0.146673011
C	4.528084326	-1.296928092	-0.455097033
H	5.604485404	-1.257304093	-0.389348030
H	4.243698308	-1.588760116	-1.460592105
H	4.155986300	-2.029484144	0.253204016
H	-0.309048023	-1.046706074	-0.599595045
O	0.851321059	3.270567234	0.538666037
H	-0.055509005	3.508980254	0.403187031
C	3.474727251	5.635230406	1.707159122
O	2.321545169	5.867303422	0.958827069
H	1.929334137	5.034718360	0.728620053
H	3.282470235	4.998233361	2.567749187
H	3.831766274	6.591618476	2.066048149
H	4.265719305	5.179431372	1.113481078
C	-4.218781304	5.547765397	-0.279759020
O	-4.532056325	4.186192299	-0.196457017
H	-3.927368282	3.756921269	0.392566030
H	-4.955301354	6.008129432	-0.923311068
H	-3.233798232	5.714759412	-0.709816052
H	-4.259971307	6.035520435	0.690712049

Coord_6

C	-2.682448191	-0.782997058	0.402840028
C	-3.811985274	-1.561079113	0.145852008
C	-4.797824343	-1.095149081	-0.716176053
C	-4.655358334	0.151494011	-1.316626096
C	-3.541012253	0.918886066	-1.072451076
C	-2.526154183	0.458988031	-0.217918017

C	0.003776002	1.015931072	-0.006459000
C	0.437862031	-0.321596022	-0.350534027
C	1.077676077	1.962560140	0.239566018
C	1.737860124	-0.683865051	-0.409528029
C	2.395673170	1.577167112	0.179245013
C	2.757670197	0.257264018	-0.129962011
H	-1.940325138	-1.134154080	1.096016080
H	-3.923742281	-2.515385182	0.627377047
H	-5.670661411	-1.690639124	-0.907340064
H	-5.417972390	0.520327040	-1.977569141
H	-3.453696250	1.884801136	-1.534951108
C	-1.361101099	1.334062094	0.054348006
O	-1.716334124	2.599550189	0.416051028
H	1.983436145	-1.691167121	-0.685679050
H	3.165111226	2.302102165	0.363284029
O	4.076082293	-0.008431000	-0.146814010
C	4.528776326	-1.296798094	-0.455303031
H	5.605178404	-1.257056089	-0.389594028
H	4.244311307	-1.588620116	-1.460785107
H	4.156714300	-2.029409144	0.252970019
H	-0.308413020	-1.047060077	-0.599646042
O	0.851264061	3.269921236	0.538766041
H	-0.055372001	3.508726255	0.403051027
C	3.474377248	5.635146404	1.707224121
O	2.321156166	5.866849420	0.958830069
H	1.929251141	5.034128364	0.728585053
H	3.282246234	4.998105359	2.567810185
H	3.831072274	6.591666472	2.066102151
H	4.265522308	5.179584373	1.113572080
C	-4.219110304	5.548644398	-0.280118019
O	-4.532776324	4.187165302	-0.196483015
H	-3.928885280	3.758143272	0.393518031
H	-4.954993357	6.008828433	-0.924503066
H	-3.233744234	5.715192412	-0.709430049
H	-4.261023306	6.036826434	0.690097050

Coord_7

C	-2.682705191	-0.783078054	0.402966030
C	-3.812295276	-1.561034112	0.145926008
C	-4.798182347	-1.094971076	-0.716018051
C	-4.655662336	0.151677011	-1.316410096
C	-3.541192252	0.918934068	-1.072313077
C	-2.526280180	0.458877030	-0.217879017
C	0.004405999	1.015259075	-0.006446998
C	0.438403030	-0.321854022	-0.350538027
C	1.077760079	1.961857144	0.239556016
C	1.738680126	-0.684061048	-0.409592028

C	2.395967171	1.576732112	0.179221015
C	2.758152199	0.257063020	-0.130050008
H	-1.940622139	-1.134265080	1.096159079
H	-3.924072281	-2.515377181	0.627359044
H	-5.671075407	-1.690381124	-0.907146063
H	-5.418299389	0.520622035	-1.977256143
H	-3.453793248	1.884835136	-1.534812109
C	-1.360803098	1.333227095	0.054393002
O	-1.716378126	2.598705188	0.416441032
H	1.984372143	-1.691323123	-0.685781049
H	3.165259226	2.301815166	0.363325024
O	4.076647295	-0.008375003	-0.146954009
C	4.529467326	-1.296668091	-0.455508034
H	5.605870403	-1.256809090	-0.389838026
H	4.244924306	-1.588480112	-1.460977103
H	4.157441300	-2.029335143	0.252737017
H	-0.307777024	-1.047414076	-0.599697044
O	0.851208064	3.269274237	0.538867040
H	-0.055235003	3.508472255	0.402914028
C	3.474028250	5.635061408	1.707288125
O	2.320768168	5.866395423	0.958832069
H	1.929168140	5.033537363	0.728551054
H	3.282023234	4.997978361	2.567871183
H	3.830379274	6.591713473	2.066154148
H	4.265326306	5.179736374	1.113663083
C	-4.219441304	5.549521398	-0.280476018
O	-4.533496328	4.188137300	-0.196508013
H	-3.930400283	3.759367270	0.394471026
H	-4.954688355	6.009524433	-0.925694069
H	-3.233693232	5.715625411	-0.709043051
H	-4.262075305	6.038131432	0.689481051

Coord_8

C	-2.682961192	-0.783158055	0.403092027
C	-3.812604274	-1.560988110	0.145999008
C	-4.798539346	-1.094793077	-0.715860050
C	-4.655966338	0.151861011	-1.316195097
C	-3.541372257	0.918982064	-1.072175078
C	-2.526406182	0.458767030	-0.217840016
C	0.005035000	1.014587073	-0.006436002
C	0.438945030	-0.322112022	-0.350541028
C	1.077845075	1.961154142	0.239546015
C	1.739501123	-0.684257050	-0.409656032
C	2.396261171	1.576297113	0.179197012
C	2.758634200	0.256862018	-0.130137010
H	-1.940919140	-1.134376080	1.096301079
H	-3.924402281	-2.515369180	0.627339047

H	-5.671488409	-1.690123123	-0.906952066
H	-5.418626389	0.520919036	-1.976943140
H	-3.453890246	1.884869135	-1.534674110
C	-1.360504097	1.332392096	0.054438004
O	-1.716423121	2.597859187	0.416830030
H	1.985307141	-1.691479124	-0.685884048
H	3.165407226	2.301528167	0.363365024
O	4.077211292	-0.008319000	-0.147094008
C	4.530158325	-1.296539093	-0.455712032
H	5.606562403	-1.256562091	-0.390082030
H	4.245538305	-1.588340113	-1.461169104
H	4.158168299	-2.029260148	0.252505021
H	-0.307142021	-1.047768074	-0.599749041
O	0.851151061	3.268627233	0.538967039
H	-0.055098004	3.508218255	0.402778030
C	3.473679248	5.634977406	1.707351124
O	2.320381165	5.865940420	0.958834070
H	1.929087139	5.032945362	0.728516054
H	3.281801239	4.997852359	2.567931186
H	3.829687274	6.591760475	2.066204150
H	4.265130309	5.179888375	1.113753080
C	-4.219774305	5.550398398	-0.280832022
O	-4.534214326	4.189107303	-0.196530017
H	-3.931914285	3.760591272	0.395425027
H	-4.954384359	6.010216433	-0.926883067
H	-3.233645231	5.716060410	-0.708656053
H	-4.263130305	6.039437436	0.688864051

Coord_9

C	-2.683218192	-0.783238056	0.403217030
C	-3.812914276	-1.560942114	0.146071008
C	-4.798895345	-1.094615078	-0.715703053
C	-4.656270334	0.152046012	-1.315980097
C	-3.541552257	0.919031066	-1.072037080
C	-2.526532179	0.458657036	-0.217802016
C	0.005664001	1.013915071	-0.006425000
C	0.439486034	-0.322370023	-0.350545023
C	1.077930077	1.960450141	0.239536019
C	1.740321126	-0.684454047	-0.409720031
C	2.396555171	1.575862113	0.179173013
C	2.759115201	0.256660020	-0.130225007
H	-1.941216140	-1.134486080	1.096442078
H	-3.924731281	-2.515360179	0.627319044
H	-5.671902411	-1.689864123	-0.906759065
H	-5.418953389	0.521216037	-1.976630142
H	-3.453986250	1.884904135	-1.534535111
C	-1.360205096	1.331558096	0.054482005

O	-1.716467123	2.597013186	0.417219028
H	1.986242144	-1.691636120	-0.685986052
H	3.165554226	2.301240167	0.363407025
O	4.077776295	-0.008263002	-0.147233012
C	4.530849325	-1.296409096	-0.455915035
H	5.607254403	-1.256315092	-0.390325028
H	4.246151304	-1.588201114	-1.461359105
H	4.158894299	-2.029186148	0.252274019
H	-0.306507025	-1.048122078	-0.599801044
O	0.851095063	3.267980235	0.539068037
H	-0.054960005	3.507964250	0.402641031
C	3.473332250	5.634892405	1.707413122
O	2.319995167	5.865484423	0.958835070
H	1.929006137	5.032353361	0.728481054
H	3.281580238	4.997725362	2.567991185
H	3.828997275	6.591807476	2.066253147
H	4.264935307	5.180040370	1.113842082
C	-4.220109306	5.551273398	-0.281189021
O	-4.534931324	4.190076301	-0.196550014
H	-3.933427283	3.761817270	0.396380028
H	-4.954084358	6.010905432	-0.928071065
H	-3.233600235	5.716496410	-0.708268049
H	-4.264187305	6.040742435	0.688247052

Coord_10

C	-2.683791195	-0.781605058	0.403071030
C	-3.813570276	-1.559124110	0.145827010
C	-4.799407345	-1.092733080	-0.716119050
C	-4.656507337	0.153805013	-1.316550095
C	-3.541633253	0.920594065	-1.072640077
C	-2.526750184	0.460127032	-0.218244017
C	0.006216002	1.014620073	-0.006567000
C	0.439881033	-0.321357024	-0.350373024
C	1.077987080	1.961067140	0.239376017
C	1.740970125	-0.683515048	-0.409317030
C	2.396794174	1.576610116	0.179299011
C	2.759468199	0.257549017	-0.129850011
H	-1.941982140	-1.132823083	1.096505077
H	-3.925580282	-2.513477181	0.627143045
H	-5.672494406	-1.687855123	-0.907175067
H	-5.419065389	0.523036036	-1.977303145
H	-3.453813251	1.886357134	-1.535305112
C	-1.359963098	1.332242095	0.054079004
O	-1.716509123	2.597789187	0.416860029
H	1.986957142	-1.690733122	-0.685388050
H	3.165684229	2.302097165	0.363591025
O	4.078188291	-0.007246003	-0.146634010

C	4.531317324	-1.295421095	-0.455058032
H	5.607715401	-1.255300088	-0.389331027
H	4.246685307	-1.587366115	-1.460483105
H	4.159207302	-2.028082147	0.253178018
H	-0.306044021	-1.047181074	-0.599667045
O	0.851085062	3.268732233	0.538732036
H	-0.054729003	3.509170250	0.401868030
C	3.473057253	5.636176406	1.707037120
O	2.319832170	5.866365424	0.958157067
H	1.929108136	5.033091362	0.727859054
H	3.281224234	4.999150362	2.567700185
H	3.828409274	6.593256475	2.065742147
H	4.264870309	5.181371373	1.113714080
C	-4.220039301	5.553875400	-0.283279022
O	-4.535386327	4.192818302	-0.198099017
H	-3.934820283	3.764874269	0.395989029
H	-4.953225355	6.013264430	-0.931204069
H	-3.233064231	5.718484413	-0.709478050
H	-4.264957305	6.043962436	0.685794050

LIIC path connecting T₂/T₁-ENOL and T1-PP-ENOL

Coord_1

C	-2.683791195	-0.781605058	0.403071030
C	-3.813570276	-1.559124110	0.145827010
C	-4.799407345	-1.092733080	-0.716119050
C	-4.656507337	0.153805013	-1.316550095
C	-3.541633253	0.920594065	-1.072640077
C	-2.526750184	0.460127032	-0.218244017
C	0.006216002	1.014620073	-0.006567000
C	0.439881033	-0.321357024	-0.350373024
C	1.077987080	1.961067140	0.239376017
C	1.740970125	-0.683515048	-0.409317030
C	2.396794174	1.576610116	0.179299011
C	2.759468199	0.257549017	-0.129850011
H	-1.941982140	-1.132823083	1.096505077
H	-3.925580282	-2.513477181	0.627143045
H	-5.672494406	-1.687855123	-0.907175067
H	-5.419065389	0.523036036	-1.977303145
H	-3.453813251	1.886357134	-1.535305112
C	-1.359963098	1.332242095	0.054079004
O	-1.716509123	2.597789187	0.416860029
H	1.986957142	-1.690733122	-0.685388050
H	3.165684229	2.302097165	0.363591025
O	4.078188291	-0.007246003	-0.146634010
C	4.531317324	-1.295421095	-0.455058032
H	5.607715401	-1.255300088	-0.389331027
H	4.246685307	-1.587366115	-1.460483105

H	4.159207302	-2.028082147	0.253178018
H	-0.306044021	-1.047181074	-0.599667045
O	0.851085062	3.268732233	0.538732036
H	-0.054729003	3.509170250	0.401868030
C	3.473057253	5.636176406	1.707037120
O	2.319832170	5.866365424	0.958157067
H	1.929108136	5.033091362	0.727859054
H	3.281224234	4.999150362	2.567700185
H	3.828409274	6.593256475	2.065742147
H	4.264870309	5.181371373	1.113714080
C	-4.220039301	5.553875400	-0.283279022
O	-4.535386327	4.192818302	-0.198099017
H	-3.934820283	3.764874269	0.395989029
H	-4.953225355	6.013264430	-0.931204069
H	-3.233064231	5.718484413	-0.709478050
H	-4.264957305	6.043962436	0.685794050

Coord_2

C	-2.672117191	-0.774895058	0.402589029
C	-3.797891273	-1.559549113	0.149385012
C	-4.789903343	-1.099155080	-0.708607051
C	-4.658226337	0.148991013	-1.308522095
C	-3.548939254	0.924360066	-1.066122079
C	-2.528445181	0.469473032	-0.216158016
C	0.003598998	1.024125075	-0.009402003
C	0.431095029	-0.316665021	-0.372405028
C	1.072345077	1.964342139	0.234199018
C	1.745023125	-0.689456047	-0.409222027
C	2.394529174	1.576792116	0.168823010
C	2.755138201	0.246264015	-0.132144010
H	-1.923595136	-1.123173081	1.090279079
H	-3.901656280	-2.515385182	0.629492047
H	-5.659120409	-1.700646120	-0.897551063
H	-5.425555388	0.512921035	-1.966682139
H	-3.469738248	1.891975134	-1.526181112
C	-1.367245101	1.352353095	0.054307006
O	-1.716122125	2.608108186	0.400716027
H	1.988593141	-1.700852123	-0.671774050
H	3.166243226	2.300317166	0.347465026
O	4.074510292	-0.012151000	-0.134686008
C	4.533459328	-1.300731093	-0.433455033
H	5.609327402	-1.257564088	-0.361424023
H	4.254736305	-1.598184117	-1.438864103
H	4.158236299	-2.030126147	0.276401020
H	-0.315015025	-1.009236075	-0.704045051
O	0.852576061	3.270296237	0.541023040
H	-0.056745005	3.508547255	0.420192030

C	3.481160253	5.622762403	1.707696121
O	2.331679168	5.864357424	0.956645070
H	1.934307139	5.034887363	0.724207053
H	3.281926236	4.985730358	2.566673184
H	3.843977277	6.576011472	2.069072148
H	4.270430305	5.162346371	1.115261082
C	-4.242711308	5.559447398	-0.280137022
O	-4.533761324	4.192455302	-0.201027013
H	-3.904485282	3.770141271	0.366010027
H	-5.004733362	6.015010435	-0.896849067
H	-3.273564235	5.745053413	-0.737612055
H	-4.262000305	6.037393436	0.695890049

Coord_3

C	-2.660321190	-0.768233055	0.401404031
C	-3.781929271	-1.560170113	0.152318009
C	-4.780287346	-1.105884082	-0.701472048
C	-4.660164338	0.143888009	-1.300684091
C	-3.556630258	0.927947068	-1.059849074
C	-2.530350182	0.478747033	-0.214569013
C	0.000508000	1.033837076	-0.012875999
C	0.421920032	-0.311364025	-0.395220029
C	1.066166075	1.967898141	0.228370019
C	1.748112128	-0.695245050	-0.409134030
C	2.391674173	1.577047116	0.157769011
C	2.750028195	0.234954016	-0.134517010
H	-1.904955137	-1.113453079	1.083138081
H	-3.877193278	-2.517506183	0.631081044
H	-5.645506404	-1.713843123	-0.888254064
H	-5.432390390	0.502433038	-1.956061139
H	-3.486300252	1.897416134	-1.517152110
C	-1.374961098	1.372542096	0.053971005
O	-1.716444124	2.618119188	0.384615026
H	1.988665141	-1.710807122	-0.657970048
H	3.166263229	2.298509163	0.330697024
O	4.069829291	-0.017259000	-0.122462008
C	4.534338328	-1.306370095	-0.410994030
H	5.609621402	-1.260323091	-0.332439022
H	4.261711306	-1.609596115	-1.416292101
H	4.155662301	-2.032181149	0.300592024
H	-0.317917023	-0.967125071	-0.807442057
O	0.853365059	3.272041236	0.542583039
H	-0.059224004	3.507878253	0.437806034
C	3.487717251	5.610189405	1.707743122
O	2.342107166	5.862872420	0.954428071
H	1.938224141	5.037182363	0.719946049
H	3.281111234	4.973347357	2.565119186

H	3.857807277	6.559653471	2.071652152
H	4.274499308	5.144179372	1.116322082
C	-4.261591304	5.563894402	-0.275455020
O	-4.530949324	4.192070304	-0.202427014
H	-3.875141277	3.774351273	0.336765025
H	-5.050523366	6.015869432	-0.860258064
H	-3.311335240	5.768542416	-0.763530056
H	-4.253895305	6.030642436	0.706196051

Coord_4

C	-2.648370192	-0.761663055	0.399550027
C	-3.765656271	-1.561010114	0.154649014
C	-4.770525343	-1.112927082	-0.694680048
C	-4.662275337	0.138487009	-1.292986092
C	-3.564650257	0.931330066	-1.053758075
C	-2.532418181	0.487907033	-0.213424016
C	-0.003003002	1.043683075	-0.016941001
C	0.412397027	-0.305493020	-0.418843031
C	1.059479074	1.971695141	0.221905018
C	1.750243125	-0.700922048	-0.409100031
C	2.388256174	1.577331115	0.146111009
C	2.744146200	0.223579018	-0.137008012
H	-1.886033135	-1.103714080	1.075105080
H	-3.852171275	-2.519864181	0.631917044
H	-5.631622407	-1.727439126	-0.879257062
H	-5.439517391	0.491578036	-1.945381141
H	-3.503436249	1.902653137	-1.508139110
C	-1.383059097	1.392745100	0.053135005
O	-1.717406121	2.627779191	0.368630026
H	1.987162146	-1.720616126	-0.644077045
H	3.165776227	2.296625165	0.313252024
O	4.064150293	-0.022594001	-0.110031010
C	4.533950325	-1.312350095	-0.387763027
H	5.608590401	-1.263583093	-0.302481023
H	4.267589306	-1.621603115	-1.392848099
H	4.151493300	-2.034268144	0.325650022
H	-0.314695021	-0.921035066	-0.909568065
O	0.853441060	3.273916233	0.543461039
H	-0.062189006	3.507077254	0.454783035
C	3.492684252	5.598474405	1.707211125
O	2.351034169	5.861907423	0.951575070
H	1.940793137	5.039961363	0.715139051
H	3.278780235	4.961990356	2.563063184
H	3.869841281	6.544207470	2.073525148
H	4.277027309	5.126920368	1.116895080
C	-4.276791307	5.567427401	-0.269371022
O	-4.526918327	4.191712300	-0.202348014

H	-3.846704276	3.777519272	0.308340020
H	-5.090703366	6.016096433	-0.821705062
H	-3.346350242	5.789295414	-0.787283055
H	-4.241019306	6.023874434	0.716550049

Coord_5

C	-2.636233189	-0.755214057	0.397055030
C	-3.749045270	-1.562086111	0.156401014
C	-4.760583341	-1.120288080	-0.688204051
C	-4.664510338	0.132781007	-1.285383095
C	-3.572949259	0.934482068	-1.047798073
C	-2.534606180	0.496914037	-0.212678014
C	-0.006886998	1.053597078	-0.021549002
C	0.402564030	-0.299082022	-0.443290030
C	1.052309077	1.975694144	0.214824013
C	1.751417126	-0.706519050	-0.409160029
C	2.384298172	1.577606112	0.133825010
C	2.737500199	0.212109016	-0.139657009
H	-1.866809136	-1.093995078	1.066203075
H	-3.826577273	-2.522473183	0.632013047
H	-5.617438403	-1.741425127	-0.870540062
H	-5.446883391	0.480358034	-1.934593138
H	-3.521082252	1.907658138	-1.499079108
C	-1.391492098	1.412906102	0.051859005
O	-1.718942122	2.637056192	0.352816024
H	1.984072142	-1.730292127	-0.630180046
H	3.164807229	2.294621165	0.295090020
O	4.057473293	-0.028174000	-0.097459008
C	4.532283327	-1.318676096	-0.363849026
H	5.606224402	-1.267344094	-0.271653019
H	4.272342307	-1.634202116	-1.368607097
H	4.145728300	-2.036397146	0.351480026
H	-0.305251022	-0.871146060	-1.010087072
O	0.852799062	3.275876237	0.543702037
H	-0.065649005	3.506068250	0.471188032
C	3.496033250	5.587622403	1.706130121
O	2.358397168	5.861455421	0.948150071
H	1.941963138	5.043211364	0.709846051
H	3.274947234	4.951640358	2.560530182
H	3.880042278	6.529684470	2.074727148
H	4.277984310	5.110603367	1.116981082
C	-4.288437307	5.570225400	-0.262008018
O	-4.521643324	4.191423300	-0.200853014
H	-3.819099273	3.779669271	0.280793021
H	-5.125409371	6.015911433	-0.781440055
H	-3.378606242	5.807630416	-0.808923060
H	-4.223732302	6.017198434	0.726831053

Coord_6

C	-2.623889188	-0.748909053	0.393950030
C	-3.732079271	-1.563409112	0.157597012
C	-4.750432340	-1.127971083	-0.682017048
C	-4.666829336	0.126759007	-1.277841092
C	-3.581479257	0.937382065	-1.041927074
C	-2.536877182	0.505739036	-0.212290016
C	-0.011103001	1.063526078	-0.026662003
C	0.392456030	-0.292152023	-0.468572034
C	1.044679076	1.979865141	0.207145016
C	1.751634126	-0.712059049	-0.409354031
C	2.379819173	1.577839114	0.120886007
C	2.730090199	0.200522013	-0.142507010
H	-1.847270134	-1.084322078	1.056460075
H	-3.800400271	-2.525338181	0.631385046
H	-5.602926405	-1.755796126	-0.862081064
H	-5.454437391	0.468767036	-1.923663141
H	-3.539180257	1.912400137	-1.489923109
C	-1.400217098	1.432980102	0.050191002
O	-1.720996123	2.645927193	0.337211026
H	1.979380144	-1.739845126	-0.616351046
H	3.163378228	2.292464165	0.276173018
O	4.049796291	-0.034006004	-0.084821006
C	4.529326327	-1.325349096	-0.339340023
H	5.602507403	-1.271598091	-0.240061016
H	4.275940310	-1.647386118	-1.343650098
H	4.138367296	-2.038571149	0.377985028
H	-0.289455023	-0.817639059	-1.108601079
O	0.851437060	3.277883237	0.543352040
H	-0.069612002	3.504786255	0.487086036
C	3.497757252	5.577627399	1.704528122
O	2.364159168	5.861507423	0.944216067
H	1.941698142	5.046915361	0.704128052
H	3.269640237	4.942270354	2.557546184
H	3.888403279	6.516084466	2.075294150
H	4.277355309	5.095241367	1.116581083
C	-4.296659309	5.572445399	-0.253478019
O	-4.515111324	4.191239300	-0.198020016
H	-3.792258271	3.780827270	0.254154016
H	-5.154793372	6.015516434	-0.739687054
H	-3.408121246	5.823838417	-0.828503058
H	-4.202375301	6.010686432	0.736942053

Coord_7

C	-2.611323186	-0.742762056	0.390265030
C	-3.714742266	-1.564981113	0.158264014

C	-4.740048343	-1.135979080	-0.676097047
C	-4.669192334	0.120409007	-1.270337094
C	-3.590200257	0.940004070	-1.036115073
C	-2.539199185	0.514356037	-0.212228017
C	-0.015619000	1.073425080	-0.032241002
C	0.382103027	-0.284715019	-0.494688037
C	1.036607075	1.984182142	0.198889015
C	1.750888123	-0.717557052	-0.409716030
C	2.374830170	1.578010113	0.107268007
C	2.721917194	0.188806013	-0.145606009
H	-1.827410133	-1.074707075	1.045908074
H	-3.773637270	-2.528454183	0.630059044
H	-5.588064404	-1.770546127	-0.853863063
H	-5.462133395	0.456795035	-1.912570135
H	-3.557677256	1.916848137	-1.480641107
C	-1.409202099	1.452926105	0.048172005
O	-1.723523124	2.654377190	0.321838025
H	1.973065144	-1.749275128	-0.602650044
H	3.161502226	2.290128165	0.256460017
O	4.041115292	-0.040089003	-0.072194006
C	4.525063328	-1.332353095	-0.314334022
H	5.597425401	-1.276326094	-0.207823014
H	4.278345310	-1.661137122	-1.318060097
H	4.129410299	-2.040778146	0.405063027
H	-0.267154018	-0.760723057	-1.204650089
O	0.849358060	3.279906234	0.542456037
H	-0.074077004	3.503175254	0.502541038
C	3.497865251	5.568473400	1.702438120
O	2.368298170	5.862050423	0.939836067
H	1.939976141	5.051056364	0.698046049
H	3.262897233	4.933845354	2.554137181
H	3.894936279	6.503395468	2.075260151
H	4.275140305	5.080835363	1.115699082
C	-4.301584309	5.574217402	-0.243888020
O	-4.507318326	4.191191304	-0.193946012
H	-3.766123270	3.781026272	0.228424016
H	-5.179016370	6.015086435	-0.696650048
H	-3.434917247	5.838182423	-0.846081061
H	-4.177262300	6.004367431	0.746812056

Coord_8

C	-2.598527188	-0.736780051	0.386033030
C	-3.697030264	-1.566804112	0.158431012
C	-4.729410340	-1.144315082	-0.670423050
C	-4.671567335	0.113715010	-1.262853093
C	-3.599076258	0.942323067	-1.030341072
C	-2.541551182	0.522744036	-0.212461014

C	-0.020408001	1.083256076	-0.038254001
C	0.371532029	-0.276779021	-0.521633039
C	1.028104075	1.988623146	0.190081013
C	1.749174124	-0.723018050	-0.410282027
C	2.369341173	1.578102115	0.092946004
C	2.712978194	0.176960015	-0.149005010
H	-1.807234128	-1.065151076	1.034583073
H	-3.746294268	-2.531813183	0.628067046
H	-5.572834402	-1.785672129	-0.845867062
H	-5.469929393	0.444423030	-1.901303137
H	-3.576527259	1.920968136	-1.471214106
C	-1.418424103	1.472714106	0.045838005
O	-1.726486125	2.662398189	0.306705022
H	1.965108144	-1.758578127	-0.589125041
H	3.159185229	2.287600163	0.235912017
O	4.031425289	-0.046408003	-0.059667005
C	4.519481328	-1.339665097	-0.288931021
H	5.590963401	-1.281492092	-0.175065010
H	4.279522306	-1.675427120	-1.291929092
H	4.118862294	-2.042994145	0.432606031
H	-0.238178018	-0.700638049	-1.297701093
O	0.846561062	3.281919235	0.541062041
H	-0.079040004	3.501189252	0.517617039
C	3.496379253	5.560138398	1.699890121
O	2.370806168	5.863067422	0.935072069
H	1.936783138	5.055617363	0.691664050
H	3.254763234	4.926325354	2.550336186
H	3.899672283	6.491592466	2.074658148
H	4.271350306	5.067369364	1.114341081
C	-4.303333308	5.575652403	-0.233338014
O	-4.498267326	4.191305299	-0.188738014
H	-3.740645270	3.780299273	0.203580012
H	-5.198231373	6.014781433	-0.652510045
H	-3.459014248	5.850899420	-0.861717064
H	-4.148665297	5.998242432	0.756390053

Coord_9

C	-2.585504184	-0.730963054	0.381287025
C	-3.678944266	-1.568870116	0.158130010
C	-4.718506341	-1.152983085	-0.664974048
C	-4.673925338	0.106660008	-1.255381089
C	-3.608077262	0.944315070	-1.024593074
C	-2.543918181	0.530886036	-0.212967013
C	-0.025457003	1.092988080	-0.044670005
C	0.360762028	-0.268348021	-0.549389042
C	1.019174072	1.993169143	0.180748014
C	1.746486125	-0.728439053	-0.411085028

C	2.363350172	1.578109111	0.077892007
C	2.703270194	0.164992010	-0.152762010
H	-1.786759128	-1.055647074	1.022528071
H	-3.718384270	-2.535397184	0.625451043
H	-5.557223398	-1.801172128	-0.838075059
H	-5.477784394	0.431626032	-1.889863134
H	-3.595687259	1.924721141	-1.461640104
C	-1.427866101	1.492318107	0.043216001
O	-1.729858122	2.669986194	0.291806020
H	1.955492141	-1.767740128	-0.575816042
H	3.156422225	2.284874165	0.214488017
O	4.020722288	-0.052934002	-0.047336006
C	4.512570326	-1.347241095	-0.263248017
H	5.583113400	-1.287044092	-0.141926010
H	4.279434309	-1.690212120	-1.265357091
H	4.106736298	-2.045180150	0.460500033
H	-0.202351014	-0.637677048	-1.387151098
O	0.843045060	3.283897236	0.539221038
H	-0.084497007	3.498784252	0.532383037
C	3.493324249	5.552590399	1.696917124
O	2.371681168	5.864541424	0.929991068
H	1.932109138	5.060579363	0.685049048
H	3.245287236	4.919664351	2.546176181
H	3.902650281	6.480648467	2.073521147
H	4.265998308	5.054820364	1.112514080
C	-4.302003311	5.576844402	-0.221920015
O	-4.487968325	4.191604300	-0.182519012
H	-3.715787269	3.778684271	0.179573013
H	-5.212573373	6.014749434	-0.607432044
H	-3.480417251	5.862202424	-0.875470063
H	-4.116815299	5.992282431	0.765638055

Coord_10

C	-2.578486188	-0.735807053	0.390876029
C	-3.664826262	-1.583054114	0.168210011
C	-4.704628340	-1.179017087	-0.660382049
C	-4.668483337	0.078489004	-1.256158091
C	-3.611395261	0.926666067	-1.023365076
C	-2.547440184	0.524556039	-0.206564016
C	-0.033370002	1.089458076	-0.026326002
C	0.351649024	-0.275816019	-0.541001037
C	1.005283074	1.986073141	0.199334016
C	1.743178127	-0.749114056	-0.360360028
C	2.353191170	1.565669112	0.104642007
C	2.690949196	0.139226010	-0.102580010
H	-1.777685130	-1.052686078	1.033468075
H	-3.698261268	-2.548139185	0.638848048

H	-5.537050399	-1.835154134	-0.834141060
H	-5.472475392	0.393670026	-1.895383136
H	-3.605607258	1.906053138	-1.462526105
C	-1.440857101	1.499104107	0.050867004
O	-1.738941127	2.665981190	0.277831021
H	1.945814140	-1.792959128	-0.502702035
H	3.148413228	2.270417164	0.237104015
O	4.006073291	-0.072519006	0.031629004
C	4.503075325	-1.369144101	-0.158121009
H	5.571480402	-1.306192096	-0.020529003
H	4.285357311	-1.725813123	-1.158858085
H	4.085593296	-2.056856149	0.568679039
H	-0.150002012	-0.594185044	-1.437738104
O	0.831180060	3.276348236	0.555861038
H	-0.098118008	3.486479251	0.556524039
C	3.471170249	5.543593401	1.720880122
O	2.359988171	5.859396424	0.940463068
H	1.917111138	5.057327363	0.695296052
H	3.209706231	4.916922356	2.570750182
H	3.883127281	6.470683466	2.096949152
H	4.246486305	5.037338364	1.147316083
C	-4.298659308	5.563532403	-0.249057018
O	-4.477743324	4.178010303	-0.207614015
H	-3.695704267	3.764223270	0.133435012
H	-5.220090378	5.998552430	-0.611517044
H	-3.494331252	5.853720421	-0.921711068
H	-4.091298292	5.978250428	0.734430054

LIIC path connecting T1-PP-ENOL and S0-ENOL

Coord_1

C	-2.578486188	-0.735807053	0.390876029
C	-3.664826262	-1.583054114	0.168210011
C	-4.704628340	-1.179017087	-0.660382049
C	-4.668483337	0.078489004	-1.256158091
C	-3.611395261	0.926666067	-1.023365076
C	-2.547440184	0.524556039	-0.206564016
C	-0.033370002	1.089458076	-0.026326002
C	0.351649024	-0.275816019	-0.541001037
C	1.005283074	1.986073141	0.199334016
C	1.743178127	-0.749114056	-0.360360028
C	2.353191170	1.565669112	0.104642007
C	2.690949196	0.139226010	-0.102580010
H	-1.777685130	-1.052686078	1.033468075
H	-3.698261268	-2.548139185	0.638848048
H	-5.537050399	-1.835154134	-0.834141060
H	-5.472475392	0.393670026	-1.895383136
H	-3.605607258	1.906053138	-1.462526105

C	-1.440857101	1.499104107	0.050867004
O	-1.738941127	2.665981190	0.277831021
H	1.945814140	-1.792959128	-0.502702035
H	3.148413228	2.270417164	0.237104015
O	4.006073291	-0.072519006	0.031629004
C	4.503075325	-1.369144101	-0.158121009
H	5.571480402	-1.306192096	-0.020529003
H	4.285357311	-1.725813123	-1.158858085
H	4.085593296	-2.056856149	0.568679039
H	-0.150002012	-0.594185044	-1.437738104
O	0.831180060	3.276348236	0.555861038
H	-0.098118008	3.486479251	0.556524039
C	3.471170249	5.543593401	1.720880122
O	2.359988171	5.859396424	0.940463068
H	1.917111138	5.057327363	0.695296052
H	3.209706231	4.916922356	2.570750182
H	3.883127281	6.470683466	2.096949152
H	4.246486305	5.037338364	1.147316083
C	-4.298659308	5.563532403	-0.249057018
O	-4.477743324	4.178010303	-0.207614015
H	-3.695704267	3.764223270	0.133435012
H	-5.220090378	5.998552430	-0.611517044
H	-3.494331252	5.853720421	-0.921711068
H	-4.091298292	5.978250428	0.734430054

Coord_2

C	-2.577807184	-0.745095055	0.388756028
C	-3.664977262	-1.591486114	0.166937012
C	-4.710644339	-1.181748086	-0.651598045
C	-4.679380335	0.080648004	-1.237927088
C	-3.621862260	0.928025069	-1.005221070
C	-2.552322183	0.520135039	-0.198437013
C	-0.037364004	1.082277077	-0.040521002
C	0.358406025	-0.269389019	-0.588281040
C	1.002900072	1.979082143	0.182094014
C	1.742056123	-0.760889054	-0.367551028
C	2.348237171	1.557546114	0.085569004
C	2.686857196	0.130456009	-0.106679006
H	-1.771864128	-1.066149078	1.023079072
H	-3.694838263	-2.560207183	0.630233043
H	-5.543633402	-1.837201134	-0.825128061
H	-5.487761396	0.399788030	-1.869611135
H	-3.619737259	1.910845139	-1.436716104
C	-1.443107105	1.491483108	0.058194003
O	-1.734498123	2.657434189	0.296513020
H	1.942582137	-1.806997131	-0.493660036
H	3.143830225	2.261914164	0.220385015

O	4.001269288	-0.076034008	0.044162006
C	4.505255323	-1.370752096	-0.139696010
H	5.572174402	-1.303303095	0.007255999
H	4.297408312	-1.729342127	-1.141881084
H	4.084544292	-2.059687147	0.584044040
H	-0.084206007	-0.525658040	-1.532243112
O	0.831420057	3.268847234	0.541960039
H	-0.098254007	3.477257248	0.553370042
C	3.447372248	5.550879399	1.723979122
O	2.353082170	5.855865420	0.915820066
H	1.915258139	5.050504363	0.672310048
H	3.167339226	4.937782354	2.577833183
H	3.852789280	6.483260464	2.094081149
H	4.233622302	5.034849363	1.174554085
C	-4.277008306	5.570550399	-0.246804020
O	-4.464260322	4.186470302	-0.193251012
H	-3.685411267	3.771003269	0.153056010
H	-5.194699374	6.007400432	-0.616458046
H	-3.468740251	5.849878420	-0.919327067
H	-4.070657294	5.993063433	0.733562055

Coord_3

C	-2.574515183	-0.753817055	0.386303027
C	-3.661670264	-1.600385113	0.165145011
C	-4.713417339	-1.185991087	-0.643381044
C	-4.688097340	0.081270005	-1.220126089
C	-3.630988260	0.928841065	-0.987318072
C	-2.555646183	0.516238040	-0.190498015
C	-0.040594002	1.078102075	-0.054664005
C	0.365007024	-0.258479019	-0.635360045
C	1.001804072	1.974460140	0.165073012
C	1.737790124	-0.770767058	-0.375100027
C	2.344203168	1.549786111	0.066448004
C	2.681660193	0.121467007	-0.111171006
H	-1.763268125	-1.078231078	1.012392072
H	-3.687143264	-2.572728184	0.620997042
H	-5.546324400	-1.841545135	-0.816827058
H	-5.501038395	0.403567027	-1.844316134
H	-3.633354260	1.915050135	-1.411050103
C	-1.444759106	1.485426108	0.065482007
O	-1.730637124	2.650044192	0.315002023
H	1.933448141	-1.819327130	-0.485618034
H	3.141209226	2.252585161	0.203636015
O	3.994661287	-0.082951005	0.056101007
C	4.502434322	-1.376918101	-0.122116011
H	5.567955399	-1.307564094	0.034073003
H	4.303498311	-1.736717127	-1.125712084

H	4.076949291	-2.066209151	0.598453044
H	-0.014881999	-0.449403033	-1.619909118
O	0.833510059	3.263688237	0.528581036
H	-0.096328008	3.470759247	0.550714038
C	3.425466247	5.559801402	1.727893123
O	2.348804169	5.854031419	0.892467067
H	1.915878139	5.045553365	0.650473046
H	3.126553223	4.960147358	2.584897186
H	3.824634277	6.497180466	2.092171153
H	4.222087302	5.034353360	1.202916086
C	-4.258665308	5.576028400	-0.245055020
O	-4.452694322	4.193355300	-0.179290015
H	-3.676618262	3.777097274	0.172293011
H	-5.173047373	6.013644432	-0.621911043
H	-3.446824248	5.845245420	-0.917394067
H	-4.053672292	6.006620430	0.732064055

Coord_4

C	-2.568636183	-0.761997056	0.383408025
C	-3.654949263	-1.609747116	0.162692010
C	-4.713007337	-1.191703085	-0.635848047
C	-4.694693338	0.080407007	-1.202815087
C	-3.638815263	0.929134065	-0.969687072
C	-2.557438184	0.512845035	-0.182803011
C	-0.043070001	1.076870077	-0.068805007
C	0.371553026	-0.243152019	-0.682223051
C	1.001967074	1.972163140	0.148197009
C	1.730396126	-0.778790057	-0.382985028
C	2.341048166	1.542401109	0.047223005
C	2.675331191	0.112274008	-0.116012010
H	-1.751911124	-1.088984076	1.001275075
H	-3.675222266	-2.585704186	0.610959042
H	-5.545197401	-1.848120135	-0.809376057
H	-5.512376399	0.405086031	-1.819537129
H	-3.646498260	1.918691139	-1.385514099
C	-1.445813105	1.480888106	0.072711007
O	-1.727338122	2.643777188	0.333340026
H	1.918425138	-1.829986131	-0.478535034
H	3.140477226	2.242465159	0.186775015
O	3.986247284	-0.093173006	0.067559006
C	4.494704323	-1.387552098	-0.105208010
H	5.558917400	-1.318813095	0.060149006
H	4.303782310	-1.747949126	-1.110180080
H	4.062898291	-2.076301148	0.612078046
H	0.058048003	-0.366076026	-1.700065120
O	0.837422060	3.260835236	0.515593036
H	-0.092371006	3.466949251	0.548411038

C	3.405447244	5.570360403	1.732395125
O	2.347144166	5.853880423	0.870179063
H	1.918955141	5.042446364	0.629590045
H	3.087365224	4.984057359	2.591742189
H	3.798669274	6.512463471	2.090958152
H	4.211853305	5.035803364	1.232176090
C	-4.243606305	5.580042400	-0.243593020
O	-4.443045320	4.198723301	-0.165585012
H	-3.669325263	3.782522272	0.191261015
H	-5.155111370	6.017402432	-0.627625046
H	-3.428533247	5.839930422	-0.915687068
H	-4.040325289	6.018937433	0.730173051

Coord_5

C	-2.560157186	-0.769648054	0.379965029
C	-3.644801263	-1.619566116	0.159441010
C	-4.709416341	-1.198861086	-0.629116045
C	-4.699186339	0.078083003	-1.186059087
C	-3.645356264	0.928909064	-0.952359067
C	-2.557698184	0.509944037	-0.175404012
C	-0.044793002	1.078560078	-0.082977004
C	0.378152025	-0.223422016	-0.728838053
C	1.003379073	1.972175142	0.131405009
C	1.719858122	-0.784956057	-0.391177030
C	2.338730169	1.535408111	0.027845000
C	2.667820192	0.102897008	-0.121162010
H	-1.737769126	-1.098431081	0.989610071
H	-3.659054261	-2.599134186	0.599937042
H	-5.540254398	-1.856889132	-0.802922058
H	-5.521801395	0.404385030	-1.795324127
H	-3.659194265	1.921776137	-1.360097096
C	-1.446260101	1.477842109	0.079871008
O	-1.724586125	2.638610190	0.351570023
H	1.897451134	-1.838941133	-0.472374035
H	3.141573226	2.231575162	0.169723014
O	3.975970286	-0.106627009	0.078638004
C	4.482051324	-1.402575101	-0.088816009
H	5.545036399	-1.336930097	0.085680004
H	4.298295308	-1.763049125	-1.095133079
H	4.042373289	-2.089835153	0.625072046
H	0.134611008	-0.276368020	-1.772053128
O	0.843161061	3.260282235	0.502887035
H	-0.086380005	3.465825252	0.546338039
C	3.387364242	5.582562400	1.737271123
O	2.348143168	5.855412423	0.848747062
H	1.924514137	5.041176365	0.609486046
H	3.049837217	5.009558363	2.598180186

H	3.774963271	6.529135470	2.090195152
H	4.202940304	5.039158363	1.262123093
C	-4.231846304	5.582633400	-0.242217016
O	-4.435333319	4.202594301	-0.152001011
H	-3.663552262	3.787275273	0.210068016
H	-5.140909369	6.018743431	-0.633372043
H	-3.413858247	5.834015422	-0.914000067
H	-4.030647288	6.030001433	0.728108053

Coord_6

C	-2.549030182	-0.776770055	0.375880029
C	-3.631164260	-1.629839119	0.155254011
C	-4.702590340	-1.207460089	-0.623313045
C	-4.701544337	0.074299005	-1.169932082
C	-3.650599262	0.928162067	-0.935366069
C	-2.556401182	0.507530037	-0.168343009
C	-0.045755004	1.083187077	-0.097188006
C	0.384923028	-0.199256015	-0.775142057
C	1.006045073	1.974508142	0.114658009
C	1.706120125	-0.789218055	-0.399636029
C	2.337212171	1.528825109	0.008271998
C	2.659052191	0.093363007	-0.126576007
H	-1.720787125	-1.106573081	0.977294069
H	-3.638555262	-2.613011188	0.587756043
H	-5.531433400	-1.867844133	-0.797620057
H	-5.529291396	0.401467030	-1.771742126
H	-3.671443263	1.924297137	-1.334792094
C	-1.446085103	1.476279104	0.086962005
O	-1.722379123	2.634526191	0.369744029
H	1.870397132	-1.846100134	-0.467102032
H	3.144450225	2.219920161	0.152402011
O	3.963723283	-0.123262008	0.089420006
C	4.464365321	-1.421923102	-0.072816007
H	5.526174399	-1.361838100	0.110821009
H	4.286955309	-1.782023129	-1.080440076
H	4.015254289	-2.106676150	0.637566048
H	0.214783017	-0.181002014	-1.835227134
O	0.850756062	3.262047237	0.490380037
H	-0.078326006	3.467420250	0.544407039
C	3.371315243	5.596427405	1.742322125
O	2.351886171	5.858638420	0.827987057
H	1.932619137	5.041752364	0.590012042
H	3.014087219	5.036715364	2.604035188
H	3.753640270	6.547226473	2.089651153
H	4.195412302	5.044388365	1.292553092
C	-4.223438302	5.583810401	-0.240748020
O	-4.429598318	4.204959305	-0.138423010

H	-3.659335264	3.791331274	0.228813014
H	-5.130495367	6.017694432	-0.638952048
H	-3.402826245	5.827558422	-0.912140067
H	-4.024724291	6.039771437	0.726071054

Coord_7

C	-2.535174183	-0.783356057	0.371072025
C	-3.613930258	-1.640563118	0.150000011
C	-4.692426338	-1.217513086	-0.618573046
C	-4.701698338	0.069032003	-1.154521086
C	-3.654499262	0.926871065	-0.918745067
C	-2.553502185	0.505595036	-0.161653013
C	-0.045940004	1.090795080	-0.111405009
C	0.391993027	-0.170585012	-0.821031059
C	1.009985073	1.979194144	0.097950005
C	1.689092122	-0.791487056	-0.408309027
C	2.336458167	1.522673111	-0.011526999
C	2.648927189	0.083708004	-0.132212009
H	-1.700884123	-1.113389080	0.964249072
H	-3.613595263	-2.627326189	0.574246042
H	-5.518604397	-1.881000135	-0.793648057
H	-5.534775398	0.396296026	-1.748882124
H	-3.683230263	1.926222141	-1.309599093
C	-1.445267106	1.476201104	0.094009005
O	-1.720722126	2.631513188	0.387929030
H	1.837069131	-1.851300131	-0.462687033
H	3.149067228	2.207492158	0.134736010
O	3.949348284	-0.143042008	0.099968007
C	4.441444321	-1.445538103	-0.057116006
H	5.502090395	-1.393491102	0.135676009
H	4.269568307	-1.804873130	-1.066008079
H	3.981332286	-2.126678156	0.649657044
H	0.298485020	-0.080737007	-1.888951134
O	0.860259064	3.266174238	0.478018033
H	-0.068155003	3.471794249	0.542570037
C	3.357444242	5.611989402	1.747360125
O	2.358496172	5.863583423	0.807733057
H	1.943365140	5.044196364	0.571041043
H	2.980285213	5.065609362	2.609144188
H	3.734880270	6.566779472	2.089100152
H	4.189374300	5.051477361	1.323268096
C	-4.218459305	5.583551400	-0.239030020
O	-4.425891320	4.205776302	-0.124758008
H	-3.656725262	3.794643273	0.247580016
H	-5.123942370	6.014239434	-0.644203047
H	-3.395490245	5.820594418	-0.909932064
H	-4.022683292	6.048182434	0.724244054

Coord_8

C	-2.518487182	-0.789392054	0.365478024
C	-3.592952259	-1.651736119	0.143552008
C	-4.678770337	-1.229049087	-0.615044042
C	-4.699531336	0.062236007	-1.139930081
C	-3.656985262	0.925000069	-0.902538067
C	-2.548933183	0.504134036	-0.155355010
C	-0.045324005	1.101450079	-0.125548011
C	0.399500030	-0.137310008	-0.866341062
C	1.015231071	1.986285145	0.081308005
C	1.668654122	-0.791630056	-0.417121030
C	2.336427168	1.516976110	-0.031570000
C	2.637323189	0.073978006	-0.138022010
H	-1.677960122	-1.118838082	0.950430068
H	-3.583996257	-2.642064188	0.559247042
H	-5.501584395	-1.896394134	-0.791200057
H	-5.538132398	0.388804030	-1.726863122
H	-3.694509263	1.927498141	-1.284526092
C	-1.443778101	1.477617108	0.101058006
O	-1.719627126	2.629561190	0.406205029
H	1.797216131	-1.854310133	-0.459092035
H	3.155385228	2.194268156	0.116652007
O	3.932643285	-0.165946011	0.110317010
C	4.412996318	-1.473362105	-0.041666004
H	5.472439392	-1.431868105	0.160284010
H	4.245824304	-1.831585130	-1.051780074
H	3.940318282	-2.149674156	0.661406049
H	0.385571027	0.023630003	-1.932603140
O	0.871741062	3.272719234	0.465792033
H	-0.055790004	3.479025250	0.540831039
C	3.345938241	5.629298403	1.752204124
O	2.368122171	5.870285421	0.787845057
H	1.956867140	5.048545365	0.552473039
H	2.948654214	5.096338368	2.613360185
H	3.718911267	6.587851474	2.088319150
H	4.184966301	5.060430363	1.354065095
C	-4.217003305	5.581808402	-0.236934017
O	-4.424271318	4.204977303	-0.110937010
H	-3.655789263	3.797147271	0.266444020
H	-5.121340368	6.008323433	-0.649005045
H	-3.391911245	5.813134421	-0.907218068
H	-4.024686291	6.055144433	0.722781053

Coord_9

C	-2.498846181	-0.794857058	0.359060025
C	-3.568051258	-1.663354121	0.135793010

C	-4.661426335	-1.242105090	-0.612883046
C	-4.694886340	0.053844002	-1.126281081
C	-3.657956265	0.922494066	-0.886789064
C	-2.542611182	0.503136034	-0.149451011
C	-0.043876001	1.115229082	-0.139479010
C	0.407588028	-0.099318008	-0.910847065
C	1.021821074	1.995842145	0.064808004
C	1.644654119	-0.789473055	-0.425976033
C	2.337072166	1.511757110	-0.051856005
C	2.624096186	0.064228005	-0.143957008
H	-1.651909117	-1.122866078	0.935831068
H	-3.549552253	-2.657202192	0.542613038
H	-5.480131396	-1.914077137	-0.790495055
H	-5.539189397	0.378893027	-1.705839121
H	-3.705210265	1.928051137	-1.259592091
C	-1.441590102	1.480536108	0.108191008
O	-1.719115125	2.628651191	0.424676030
H	1.750538126	-1.854823134	-0.456278035
H	3.163362226	2.180214155	0.098076007
O	3.913361283	-0.191959015	0.120473011
C	4.378652313	-1.505327109	-0.026470002
H	5.436785392	-1.476957107	0.184606013
H	4.215302302	-1.862119133	-1.037751077
H	3.891858282	-2.175469155	0.672832050
H	0.475834034	0.131260009	-1.965566142
O	0.885286063	3.281749236	0.453735031
H	-0.041140001	3.489199249	0.539256038
C	3.337019239	5.648418408	1.756682127
O	2.380928170	5.878786420	0.768198056
H	1.973254140	5.054841362	0.534236041
H	2.919472211	5.129020370	2.616546187
H	3.705999268	6.610515474	2.087089151
H	4.182364299	5.071266362	1.384738097
C	-4.219169302	5.578502404	-0.234365015
O	-4.424796320	4.202465303	-0.096923010
H	-3.656595264	3.798757271	0.285462021
H	-5.122767369	5.999856433	-0.653289047
H	-3.392148242	5.805159418	-0.903862063
H	-4.030916289	6.060541438	0.721807049

Coord_10

C	-2.495403179	-0.784348058	0.383046026
C	-3.555586255	-1.662881121	0.156119010
C	-4.655586335	-1.247907090	-0.586536041
C	-4.704632340	0.051733003	-1.090059079
C	-3.677123267	0.930044065	-0.846250059
C	-2.555387183	0.517088036	-0.114793008

C	-0.063991002	1.152610084	-0.117662011
C	0.399085028	-0.036183002	-0.915823067
C	1.004707075	2.031166144	0.085667007
C	1.599824116	-0.760871057	-0.391817028
C	2.314765165	1.533206109	-0.030784003
C	2.589171186	0.081224003	-0.105440006
H	-1.642773116	-1.107157081	0.954657067
H	-3.525374255	-2.659514189	0.555286040
H	-5.467262393	-1.927478138	-0.767370057
H	-5.553908399	0.371533029	-1.665260122
H	-3.736418271	1.937859140	-1.211194085
C	-1.462696103	1.502445110	0.146326008
O	-1.746886125	2.646054190	0.471765037
H	1.682192122	-1.828356133	-0.409442027
H	3.147376226	2.193654157	0.121930011
O	3.871148280	-0.190908011	0.179007011
C	4.321430313	-1.510325109	0.040256000
H	5.377397385	-1.494890110	0.263361018
H	4.164680302	-1.867262133	-0.972053071
H	3.818590274	-2.172976159	0.735294052
H	0.553923038	0.260413019	-1.948816142
O	0.871722064	3.316845240	0.476744033
H	-0.054130006	3.523860253	0.569829042
C	3.292251235	5.700649409	1.798847129
O	2.360778169	5.916639427	0.783921055
H	1.958977139	5.089335368	0.551586037
H	2.853114204	5.195245374	2.656301189
H	3.654536262	6.667422481	2.123015154
H	4.145453297	5.116762366	1.456597103
C	-4.257737306	5.583869404	-0.214528018
O	-4.457376319	4.208210300	-0.064509003
H	-3.689251263	3.811854276	0.325671025
H	-5.160731370	5.996285429	-0.643507047
H	-3.427552248	5.807939419	-0.880968061
H	-4.078156292	6.076420438	0.737935054

Coord_11

C	-2.530529182	-0.775304054	0.399456029
C	-3.599312261	-1.643733117	0.177792014
C	-4.687316338	-1.228072088	-0.582458042
C	-4.715879341	0.061104007	-1.108384079
C	-3.677579264	0.931656066	-0.871617065
C	-2.567797183	0.517873039	-0.123662008
C	-0.066714006	1.128936080	-0.101624009
C	0.390569027	-0.085156007	-0.859124063
C	0.996706073	2.012114144	0.118988007
C	1.632039115	-0.763281057	-0.389711029

C	2.311498168	1.534386111	0.017152000
C	2.606250186	0.099615008	-0.092168008
H	-1.688784120	-1.098548077	0.986424070
H	-3.585400260	-2.633408187	0.594818041
H	-5.505866397	-1.900758137	-0.758186054
H	-5.556210400	0.382040028	-1.695930124
H	-3.720977270	1.933292140	-1.255178092
C	-1.467229105	1.496724106	0.131300009
O	-1.745478127	2.647323189	0.435786032
H	1.754241128	-1.826213134	-0.435913029
H	3.133035226	2.204693159	0.185260012
O	3.898348281	-0.145665013	0.170010013
C	4.380707314	-1.451274104	0.010049002
H	5.437700393	-1.411170104	0.224829014
H	4.225894303	-1.799397130	-1.005592071
H	3.901108279	-2.135615155	0.700554053
H	0.398217030	0.089703005	-1.916631137
O	0.852712060	3.297262237	0.507602036
H	-0.074842004	3.504838252	0.577704041
C	3.309460238	5.669906407	1.796185130
O	2.346065169	5.897101425	0.814118057
H	1.938410141	5.072023366	0.584090041
H	2.899289211	5.149556369	2.659028193
H	3.677745267	6.633194477	2.123875151
H	4.153978300	5.095143369	1.418746102
C	-4.252847306	5.588975404	-0.226654019
O	-4.453366319	4.211756301	-0.093608005
H	-3.683668263	3.809890272	0.287639019
H	-5.157900372	6.008311432	-0.644493047
H	-3.426512245	5.820816418	-0.895215063
H	-4.066608295	6.068692434	0.731093052

Coord_12

C	-2.561584187	-0.765681056	0.414351030
C	-3.638139260	-1.624677116	0.197425014
C	-4.714358338	-1.209458087	-0.580147041
C	-4.723520338	0.068805007	-1.127635082
C	-3.675181265	0.932122065	-0.897416065
C	-2.577119185	0.518624036	-0.133241010
C	-0.067319003	1.107409081	-0.085953006
C	0.384319025	-0.128347010	-0.801555056
C	0.990576074	1.995358143	0.151837013
C	1.659685118	-0.761684053	-0.387656028
C	2.309101164	1.536107112	0.064033003
C	2.621426191	0.118730007	-0.079157005
H	-1.730592123	-1.088382079	1.016429076
H	-3.639739259	-2.607020187	0.631700044

H	-5.539178401	-1.875724137	-0.751153055
H	-5.555074399	0.390054026	-1.727342122
H	-3.703465265	1.927158139	-1.298995095
C	-1.469477108	1.491610105	0.116017011
O	-1.742821123	2.648439192	0.399797031
H	1.816555131	-1.818477129	-0.463465034
H	3.120189226	2.215007157	0.246975018
O	3.921919281	-0.104673006	0.160035011
C	4.430157319	-1.397522099	-0.021921003
H	5.487874397	-1.337214096	0.184147015
H	4.274887306	-1.735765127	-1.040796074
H	3.971766285	-2.101120149	0.663693047
H	0.252581016	-0.079511004	-1.852439132
O	0.835115059	3.279902238	0.537756038
H	-0.093652006	3.487688252	0.584782041
C	3.326336240	5.642763408	1.791356128
O	2.332067166	5.880203425	0.843158061
H	1.918921136	5.057139362	0.615727046
H	2.945374210	5.107488365	2.658451194
H	3.700470265	6.602654478	2.122300151
H	4.161232299	5.077794367	1.379298097
C	-4.249100308	5.591851403	-0.237222017
O	-4.449382318	4.213086304	-0.121569011
H	-3.677746267	3.806353272	0.250393016
H	-5.156584372	6.017301434	-0.643504046
H	-3.426955246	5.832429419	-0.907857065
H	-4.056411293	6.058512435	0.725710054

Coord_13

C	-2.588584186	-0.755447054	0.427821031
C	-3.672029263	-1.605815117	0.215178017
C	-4.736726342	-1.192255085	-0.579446040
C	-4.727669341	0.074693004	-1.147728085
C	-3.670103265	0.931440066	-0.923628066
C	-2.583478187	0.519429037	-0.143505012
C	-0.065887007	1.088365076	-0.070689005
C	0.379985027	-0.165461010	-0.743224054
C	0.986345069	1.981101145	0.184244013
C	1.682713123	-0.756176053	-0.385661029
C	2.307714164	1.538451113	0.110001006
C	2.634870188	0.138518008	-0.066363002
H	-1.768168126	-1.076565080	1.044760077
H	-3.688271264	-2.580493188	0.666145048
H	-5.567172401	-1.852675134	-0.746061053
H	-5.550656399	0.395363029	-1.759416127
H	-3.684141263	1.919493139	-1.342676094
C	-1.469637104	1.487334109	0.100428010

O	-1.739215124	2.649662189	0.363696025
H	1.869073136	-1.805652132	-0.492000034
H	3.109060221	2.224656159	0.307343024
O	3.942221282	-0.068390005	0.149070009
C	4.469928323	-1.349985096	-0.055667002
H	5.528341396	-1.274192092	0.141254008
H	4.311781311	-1.677285119	-1.077638077
H	4.030315292	-2.070523147	0.624706046
H	0.119369010	-0.243397018	-1.758434128
O	0.818971057	3.264950235	0.567269041
H	-0.110511006	3.472625248	0.591061041
C	3.342972239	5.619195404	1.784779127
O	2.318997165	5.866006425	0.871319064
H	1.900680137	5.044782364	0.646706045
H	2.991314214	5.069059365	2.654949189
H	3.722849266	6.575744476	2.118769152
H	4.167317298	5.064604365	1.338762098
C	-4.246982308	5.592533401	-0.246489016
O	-4.445825321	4.212247304	-0.148567010
H	-3.671849264	3.801376275	0.213770013
H	-5.157307371	6.023191436	-0.640810047
H	-3.429414248	5.842820423	-0.919160064
H	-4.048035290	6.046003436	0.721485050

Coord_14

C	-2.611453189	-0.744547055	0.440021032
C	-3.700816268	-1.587278112	0.231255014
C	-4.754289344	-1.176745085	-0.580202043
C	-4.728321341	0.078520008	-1.168614087
C	-3.662439265	0.929551068	-0.950245068
C	-2.586930184	0.520382037	-0.154397009
C	-0.062466003	1.072253079	-0.055756004
C	0.377242026	-0.196048016	-0.684080051
C	0.984098071	1.969640140	0.216361013
C	1.701008125	-0.746651053	-0.383688029
C	2.307517167	1.541551112	0.155279010
C	2.646759192	0.159000009	-0.053723006
H	-1.801408130	-1.062932077	1.071607075
H	-3.730730266	-2.553981185	0.698436053
H	-5.589641400	-1.832035132	-0.742722055
H	-5.542979397	0.397600030	-1.792142131
H	-3.663202264	1.910262139	-1.386294101
C	-1.467888105	1.484181107	0.084535007
O	-1.734992126	2.651293193	0.327392026
H	1.911615140	-1.787991127	-0.521412039
H	3.099930226	2.233720161	0.366708028
O	3.959560283	-0.037343001	0.137015007

C	4.499940325	-1.309630092	-0.091364008
H	5.559271399	-1.223457091	0.095843006
H	4.336381311	-1.624840119	-1.116251082
H	4.076258292	-2.044876148	0.583432041
H	0.000235002	-0.398292030	-1.636987118
O	0.804410057	3.252684234	0.596335044
H	-0.125266008	3.459980251	0.596691042
C	3.359639243	5.599192404	1.776988130
O	2.307223167	5.854630421	0.899013063
H	1.883992135	5.035119360	0.677362050
H	3.037228220	5.034294362	2.649027192
H	3.745227267	6.552408473	2.113879152
H	4.172505298	5.055475364	1.297741093
C	-4.247103304	5.590983404	-0.254867019
O	-4.443170317	4.209205302	-0.174902013
H	-3.666412264	3.795051274	0.177523012
H	-5.160720374	6.025796432	-0.636880044
H	-3.434534250	5.851964421	-0.929526069
H	-4.042125290	6.031243434	0.717960053

Coord_15

C	-2.629986188	-0.732893053	0.451166034
C	-3.724139268	-1.569241111	0.245889019
C	-4.766704345	-1.163351085	-0.582293040
C	-4.725303342	0.079881004	-1.190302088
C	-3.652182264	0.926317064	-0.977295069
C	-2.587453186	0.521593038	-0.165827010
C	-0.057071004	1.059729078	-0.040932003
C	0.375787026	-0.219391014	-0.623893044
C	0.984009069	1.961432140	0.248494016
C	1.714341121	-0.732752054	-0.381645029
C	2.308763168	1.545618110	0.200181017
C	2.657268191	0.180288011	-0.041148003
H	-1.830095131	-1.047212073	1.097269076
H	-3.766623269	-2.527676181	0.728901051
H	-5.606117402	-1.814427129	-0.741000054
H	-5.531884397	0.396166029	-1.825616132
H	-3.640781262	1.899337138	-1.429975100
C	-1.464405108	1.482536107	0.068400007
O	-1.730571125	2.653708189	0.290807024
H	1.943781142	-1.765446128	-0.551600040
H	3.093192222	2.242296161	0.425503033
O	3.974144286	-0.012171003	0.123663008
C	4.519769327	-1.277532094	-0.129394008
H	5.580460402	-1.186648087	0.047302006
H	4.348040314	-1.579307115	-1.156955084
H	4.108704297	-2.025282148	0.539518039

H	-0.103811008	-0.540669037	-1.490445105
O	0.791709057	3.243554233	0.625319045
H	-0.137603008	3.450293249	0.602024043
C	3.376908244	5.582760402	1.768662129
O	2.297401166	5.846282422	0.926820068
H	1.869398136	5.028429364	0.708203051
H	3.083524223	5.003220360	2.641344190
H	3.768300274	6.532577471	2.108380154
H	4.177347302	5.050293364	1.256952090
C	-4.250320305	5.587052400	-0.262952017
O	-4.442046318	4.203801301	-0.201032013
H	-3.662017262	3.787407271	0.141297009
H	-5.167732374	6.024751434	-0.632428044
H	-3.443202247	5.859761424	-0.939511067
H	-4.039642290	6.014247435	0.714496053

Coord_16

C	-2.643777188	-0.720340054	0.461514032
C	-3.741317272	-1.551965109	0.259305017
C	-4.773286341	-1.152732086	-0.585680044
C	-4.718198339	0.078119008	-1.212906085
C	-3.639201261	0.921490068	-1.004856070
C	-2.584916189	0.523221036	-0.177686015
C	-0.049695004	1.051842078	-0.025815002
C	0.375306025	-0.234320019	-0.562228041
C	0.986384069	1.957219143	0.281129023
C	1.722272123	-0.713772054	-0.379361026
C	2.311805165	1.550980109	0.245131015
C	2.666535191	0.202608014	-0.028521003
H	-1.853825132	-1.028961073	1.122143079
H	-3.795059275	-2.501844182	0.757882052
H	-5.615700405	-1.800825131	-0.740884053
H	-5.516957396	0.390095027	-1.860097136
H	-3.616969260	1.886470135	-1.473921106
C	-1.459393106	1.482976107	0.052149005
O	-1.726549124	2.657440190	0.253876018
H	1.964753140	-1.737596128	-0.582445041
H	3.089426221	2.250492164	0.484270035
O	3.986004286	0.006303999	0.108667008
C	4.528425328	-1.254967093	-0.170372013
H	5.591095404	-1.165875086	-0.005343002
H	4.345403312	-1.541617111	-1.200282085
H	4.126092294	-2.012943143	0.492388037
H	-0.192352014	-0.666956050	-1.320900096
O	0.781419057	3.238306234	0.654810045
H	-0.146915009	3.444502250	0.607670042
C	3.395915243	5.569887398	1.760674124

O	2.290742164	5.841297419	0.955555070
H	1.857906136	5.025179363	0.739964052
H	3.131134226	4.975836358	2.632748187
H	3.793438273	6.516109470	2.103221152
H	4.182893302	5.048878365	1.217259086
C	-4.257989306	5.580415401	-0.271576018
O	-4.443410320	4.195681304	-0.227617016
H	-3.659537262	3.778384270	0.104597006
H	-5.179785371	6.019392435	-0.628473047
H	-3.456805251	5.866008420	-0.949867066
H	-4.042155289	5.994914431	0.710229053

Coord_17

C	-2.652058193	-0.706638051	0.471330032
C	-3.751084270	-1.535882111	0.271641017
C	-4.772746342	-1.145999083	-0.590514041
C	-4.706197340	0.072126007	-1.236749086
C	-3.623203259	0.914646065	-1.033126073
C	-2.579041183	0.525529038	-0.189873014
C	-0.040340002	1.050423073	-0.009756002
C	0.375389027	-0.238828017	-0.498421033
C	0.991761071	1.958281138	0.315000023
C	1.723954123	-0.688486049	-0.376553026
C	2.317160168	1.558165114	0.290687022
C	2.674572192	0.226349017	-0.015678003
H	-1.871853137	-1.007419071	1.146714081
H	-3.814400275	-2.476926178	0.785645056
H	-5.616709403	-1.792867130	-0.742622051
H	-5.497379394	0.377750025	-1.896136134
H	-3.591857259	1.871229137	-1.518464109
C	-1.453174104	1.486470106	0.035988001
O	-1.723927125	2.663327192	0.216557015
H	1.972917144	-1.703508122	-0.613783044
H	3.089566220	2.258401163	0.543672038
O	3.994796286	0.016924999	0.091535006
C	4.523944324	-1.243566091	-0.215150018
H	5.589306404	-1.164039085	-0.063454004
H	4.325972310	-1.512857111	-1.246948089
H	4.125667296	-2.009243146	0.441254031
H	-0.265528020	-0.773062057	-1.129951079
O	0.774624056	3.238268234	0.685707048
H	-0.152015013	3.444340248	0.614617043
C	3.418922245	5.560467398	1.754161127
O	2.289615164	5.840225422	0.986379074
H	1.851479136	5.026161363	0.773714056
H	3.182015227	4.952034357	2.624338190
H	3.823372274	6.502654466	2.099640151

H	4.191185303	5.050825362	1.179729084
C	-4.272500309	5.570424402	-0.281874019
O	-4.448913319	4.184130301	-0.255607021
H	-3.660475266	3.767756269	0.066735003
H	-5.199423376	6.008501433	-0.626452045
H	-3.477789251	5.870339423	-0.961594068
H	-4.052449290	5.972903431	0.704011051

Coord_18

C	-2.653349189	-0.691333049	0.480790033
C	-3.750973270	-1.521805107	0.282770022
C	-4.762591341	-1.145187082	-0.597383042
C	-4.687763339	0.059903002	-1.262578090
C	-3.603658261	0.905053066	-1.062547074
C	-2.569318187	0.529028037	-0.202359015
C	-0.029111004	1.059005074	0.008274999
C	0.375253028	-0.229273018	-0.431559033
C	1.001118073	1.967017140	0.351190026
C	1.717695126	-0.654829048	-0.372747025
C	2.325612166	1.568063115	0.337581022
C	2.681020191	0.252118018	-0.002363999
H	-1.882730137	-0.981209070	1.171501082
H	-3.821442275	-2.453777176	0.812177056
H	-5.605882405	-1.793559130	-0.747036056
H	-5.471609393	0.356187026	-1.934840137
H	-3.565687259	1.852889134	-1.564181113
C	-1.446415103	1.494835107	0.020217000
O	-1.724646123	2.672885191	0.178836012
H	1.965030143	-1.661478119	-0.645298047
H	3.095216225	2.266020162	0.604506043
O	3.999355285	0.017923001	0.071676005
C	4.502521324	-1.245629088	-0.264703017
H	5.571213400	-1.185453083	-0.128685011
H	4.285232308	-1.494478108	-1.297718095
H	4.102397293	-2.015888146	0.385263030
H	-0.324139025	-0.853208063	-0.918471064
O	0.773548053	3.245995233	0.719401050
H	-0.150487013	3.453267246	0.624458047
C	3.450633250	5.554074402	1.750672124
O	2.298922165	5.843997419	1.021019075
H	1.854170134	5.032812364	0.811061058
H	3.240298232	4.931367355	2.617576188
H	3.863796277	6.491276468	2.099322153
H	4.206399302	5.055112364	1.145722080
C	-4.298508307	5.555768399	-0.295421020
O	-4.461757319	4.167707301	-0.286393018
H	-3.667736265	3.754980269	0.026721001

H	-5.231612376	5.989722430	-0.628401047
H	-3.510938252	5.872099425	-0.976008073
H	-4.075922296	5.947336428	0.694307052

Coord_19

C	-2.637431189	-0.695595048	0.436158033
C	-3.736978267	-1.523800110	0.243698019
C	-4.750410342	-1.147863083	-0.635095044
C	-4.675607339	0.053070006	-1.303631095
C	-3.587005259	0.897287067	-1.110708078
C	-2.550899183	0.522000039	-0.253248017
C	-0.005549000	1.052874074	-0.040131003
C	0.369371027	-0.227380018	-0.454634034
C	1.038664077	1.944421139	0.317609020
C	1.693231124	-0.646326048	-0.487964036
C	2.357777168	1.530150110	0.286557021
C	2.689447195	0.231993015	-0.111990009
H	-1.867100136	-0.984384070	1.127377082
H	-3.807979275	-2.453741176	0.776626055
H	-5.595569402	-1.795063131	-0.779434055
H	-5.461169393	0.349656026	-1.973727140
H	-3.548627256	1.843053131	-1.616089115
C	-1.427195105	1.488841106	-0.036476003
O	-1.709663126	2.665927193	0.120122008
H	1.916141140	-1.642602117	-0.814793060
H	3.137568227	2.211928161	0.564997040
O	4.000131287	-0.051352006	-0.099748006
C	4.445979322	-1.319964093	-0.493115037
H	5.520039399	-1.300779094	-0.392400028
H	4.186598299	-1.527752112	-1.525463108
H	4.041023289	-2.096791151	0.146030013
H	-0.383459028	-0.916571064	-0.778715057
O	0.819464060	3.219030233	0.705953052
H	-0.100960008	3.438381246	0.605170044
C	3.567884255	5.470021396	1.689361124
O	2.387378174	5.792071415	1.022001074
H	1.924343139	4.991646359	0.810230059
H	3.390906242	4.822152346	2.545209183
H	4.005295289	6.392334462	2.047926146
H	4.290869311	4.984147356	1.035644073
C	-4.311069308	5.532672400	-0.254039016
O	-4.462977321	4.143584296	-0.278974022
H	-3.659670265	3.729799269	0.007872999
H	-5.254252378	5.967519428	-0.556090040
H	-3.540258255	5.873784420	-0.941803066
H	-4.071159293	5.899610424	0.741088051

LIIC path connecting T1-PP-KETO and S0-KETO

Coord_1

C	-2.644569192	-0.728275051	0.387187028
C	-3.731929270	-1.539068112	0.153002013
C	-4.757312343	-1.121638080	-0.687622051
C	-4.685233337	0.131623009	-1.286621095
C	-3.588897259	0.956337067	-1.053740078
C	-2.542022182	0.531436037	-0.223420016
C	-0.024544003	1.053438076	-0.028619001
C	0.407289027	-0.223071018	-0.378902028
C	1.053265078	2.024341144	0.263039019
C	1.806889131	-0.627978044	-0.403566027
C	2.415889175	1.594235116	0.219114016
C	2.778613202	0.245426016	-0.114776011
H	-1.879779133	-1.054533076	1.068138075
H	-3.796532272	-2.497316182	0.636248047
H	-5.604355401	-1.758799128	-0.859599063
H	-5.475024396	0.469498036	-1.931817138
H	-3.549549258	1.926971139	-1.507620109
C	-1.401666102	1.430838104	0.021825000
O	-1.782582126	2.731372194	0.146876008
H	2.019257148	-1.646301119	-0.664962046
H	3.181782230	2.311863168	0.437956029
O	4.103368296	0.022504003	-0.090893008
C	4.578089327	-1.258793092	-0.399694027
H	5.652243407	-1.209961086	-0.312042023
H	4.310949312	-1.542177113	-1.412130100
H	4.193362301	-1.996792145	0.295919024
H	-0.309556022	-0.960684068	-0.673054050
O	0.821174059	3.221138232	0.535095038
H	-1.028187071	3.287926238	0.300659023
C	3.429554247	5.558772401	1.737109126
O	2.278880164	5.929631427	1.042281072
H	1.801987130	5.150099368	0.792734057
H	3.208504231	4.900366353	2.574527185
H	3.881163277	6.460897465	2.126710155
H	4.157675297	5.066121362	1.094222079
C	-4.298487309	5.548618399	-0.269717019
O	-4.535530327	4.174030303	-0.213512013
H	-3.747636267	3.723205270	0.062874004
H	-5.213506376	6.023369435	-0.597957041
H	-3.509881253	5.802358419	-0.975643073
H	-4.034928289	5.959594427	0.702422048

Coord_2

C	-2.637917190	-0.717027050	0.380929026
C	-3.732423268	-1.519495111	0.162754014

C	-4.773681346	-1.091106077	-0.655563049
C	-4.707395339	0.166280012	-1.245476087
C	-3.603207259	0.985175068	-1.027278072
C	-2.540752183	0.548854038	-0.221299015
C	-0.011226003	1.052382077	-0.040472005
C	0.425871028	-0.209649014	-0.414833031
C	1.054609077	2.019822145	0.293159021
C	1.827463130	-0.612596047	-0.423807031
C	2.418812176	1.595997117	0.265808018
C	2.790842202	0.255879018	-0.095386009
H	-1.860136132	-1.053511076	1.041767077
H	-3.791917274	-2.481574180	0.638895045
H	-5.626036406	-1.724031124	-0.816631056
H	-5.507702399	0.511946037	-1.873384137
H	-3.567981258	1.958441140	-1.475476104
C	-1.395059102	1.441826104	-0.001973000
O	-1.745594123	2.756895196	0.051534006
H	2.047279147	-1.624162116	-0.704354048
H	3.179135227	2.308804169	0.517436039
O	4.115130298	0.035269002	-0.052556006
C	4.598801330	-1.237839091	-0.381559027
H	5.671030406	-1.188773083	-0.272893019
H	4.351077315	-1.498452107	-1.404949102
H	4.202954300	-1.992125146	0.289861019
H	-0.285911023	-0.942270070	-0.734076050
O	0.808538057	3.210766231	0.580010042
H	-0.983055073	3.295369237	0.228412015
C	3.472619247	5.491164398	1.728606126
O	2.291128167	5.903114424	1.113111082
H	1.786418126	5.139960369	0.867372063
H	3.287244234	4.820646345	2.565175184
H	3.968837284	6.374324459	2.107241152
H	4.148051298	4.995501357	1.032750077
C	-4.382576315	5.521229397	-0.307351020
O	-4.556907331	4.139149299	-0.212116017
H	-3.734462267	3.728291267	0.021476002
H	-5.336068383	5.950744430	-0.584434043
H	-3.651981262	5.793106417	-1.066871077
H	-4.075631291	5.962319430	0.638477048

Coord_3

C	-2.629287188	-0.705492049	0.374575025
C	-3.728391271	-1.502918109	0.173343015
C	-4.785162343	-1.068272079	-0.624646042
C	-4.726856340	0.191833013	-1.208529085
C	-3.617378261	1.008272073	-1.006007073
C	-2.539675185	0.565346043	-0.222410017

C	-0.000526002	1.053040077	-0.053415003
C	0.441697032	-0.193780015	-0.452988034
C	1.053095074	2.014533146	0.324184021
C	1.844641134	-0.596350041	-0.445264030
C	2.418154176	1.595336117	0.314427025
C	2.799267202	0.264846022	-0.075176005
H	-1.838959130	-1.048516077	1.016770072
H	-3.781186274	-2.467703179	0.644677047
H	-5.640908404	-1.699477120	-0.774097054
H	-5.537463396	0.541643040	-1.820765133
H	-3.588073256	1.983073145	-1.450929106
C	-1.390973102	1.453658105	-0.028459004
O	-1.713930125	2.777801201	-0.050908005
H	2.071688151	-1.600449117	-0.745943051
H	3.172630226	2.301403164	0.600370041
O	4.122480295	0.044874003	-0.012224000
C	4.614731333	-1.219489087	-0.362367028
H	5.684543407	-1.171799083	-0.231471019
H	4.387501315	-1.455343106	-1.396421098
H	4.206864301	-1.990114145	0.282722021
H	-0.264861018	-0.919772068	-0.799121057
O	0.793552059	3.199113229	0.626692043
H	-0.948402070	3.303893235	0.149316013
C	3.507770253	5.431488391	1.717030125
O	2.298968166	5.876422422	1.182870085
H	1.768811129	5.127359368	0.947186069
H	3.361343242	4.751742340	2.553983185
H	4.044716290	6.298702453	2.076469151
H	4.128077296	4.933640357	0.973112071
C	-4.449330321	5.499890398	-0.335288023
O	-4.570883330	4.114644296	-0.206934017
H	-3.721559270	3.735314269	-0.022159001
H	-5.433043389	5.893223424	-0.554410040
H	-3.780569275	5.781486414	-1.146434083
H	-4.094893295	5.967541431	0.580673043

Coord_4

C	-2.618406187	-0.694505049	0.368365024
C	-3.719548269	-1.490280108	0.185195014
C	-4.791942342	-1.054136077	-0.594116045
C	-4.744316342	0.207376012	-1.174892087
C	-3.632147259	1.024847074	-0.989255073
C	-2.539052185	0.580185041	-0.226416016
C	0.007439999	1.054645077	-0.067453007
C	0.454881033	-0.176005014	-0.493506035
C	1.048407077	2.007674146	0.355925025
C	1.858544134	-0.579651043	-0.468415032

C	2.413617174	1.591580117	0.364456024
C	2.803816200	0.271851021	-0.054809004
H	-1.815581132	-1.040364075	0.993169074
H	-3.763652272	-2.456717179	0.653932045
H	-5.649126405	-1.686233120	-0.731075054
H	-5.565369399	0.557648038	-1.772807127
H	-3.610948260	2.000144144	-1.433192101
C	-1.389511102	1.465517105	-0.057469004
O	-1.687307122	2.792954202	-0.159492012
H	2.092775150	-1.575432114	-0.790299059
H	3.161811229	2.288938167	0.686099047
O	4.125329295	0.050945005	0.029132001
C	4.625988335	-1.203938086	-0.343259025
H	5.692839409	-1.159186085	-0.189160012
H	4.420235320	-1.412972101	-1.387489099
H	4.205496304	-1.990935142	0.273257019
H	-0.246151020	-0.893682063	-0.868209063
O	0.775741054	3.185284230	0.675079047
H	-0.923805065	3.312522238	0.064557005
C	3.533398255	5.381255389	1.703782125
O	2.300052164	5.849713422	1.252245090
H	1.748392127	5.111370367	1.032145074
H	3.430345245	4.694776340	2.541817184
H	4.105245293	6.236659448	2.036715145
H	4.097426297	4.882484353	0.916954067
C	-4.496720324	5.487194394	-0.355241027
O	-4.576310329	4.101773298	-0.197740012
H	-3.707653264	3.744870268	-0.066502007
H	-5.502428396	5.854260420	-0.510952035
H	-3.893027283	5.770115417	-1.215438087
H	-4.090558296	5.978101428	0.526399037

Coord_5

C	-2.605043186	-0.684835049	0.362586028
C	-3.705591267	-1.482466107	0.198864016
C	-4.794124346	-1.049735074	-0.563068041
C	-4.760373342	0.211876014	-1.143590083
C	-3.648210260	1.033998073	-0.976347069
C	-2.539169181	0.592618045	-0.233002019
C	0.012486001	1.056445078	-0.082667006
C	0.465454032	-0.156837013	-0.536537041
C	1.040174074	1.998470145	0.388058028
C	1.869232133	-0.562866038	-0.493755034
C	2.404864175	1.584092116	0.415239032
C	2.804367200	0.276469019	-0.035021003
H	-1.789429129	-1.029728073	0.971008067
H	-3.738622267	-2.449504176	0.667171049

H	-5.650717408	-1.685431120	-0.686432048
H	-5.592331404	0.558824039	-1.728254122
H	-3.637676262	2.008737147	-1.421530103
C	-1.390855101	1.476589107	-0.088930004
O	-1.665577120	2.801236201	-0.273433018
H	2.110766150	-1.549329113	-0.837970060
H	3.146190229	2.270730162	0.773776055
O	4.123554297	0.053172005	0.070452002
C	4.632649333	-1.191303085	-0.325419026
H	5.695955411	-1.150990082	-0.147405011
H	4.449234318	-1.371423098	-1.379115097
H	4.199237301	-1.994646146	0.260221018
H	-0.229611019	-0.864474061	-0.941324065
O	0.754564052	3.168397226	0.724927052
H	-0.909273064	3.320357241	-0.024854000
C	3.547873253	5.341929386	1.690415123
O	2.292003167	5.823098421	1.322047093
H	1.724313122	5.091080367	1.121944082
H	3.493488252	4.650904334	2.529401182
H	4.146897300	6.190717443	1.990915145
H	4.055985294	4.843908347	0.865941062
C	-4.522527325	5.485613397	-0.368902028
O	-4.571687330	4.102070293	-0.184075015
H	-3.691279266	3.757813272	-0.110139010
H	-5.541885397	5.837236418	-0.456743033
H	-3.986964288	5.761461416	-1.275234089
H	-4.060118290	5.996371431	0.472813035

Coord_6

C	-2.589018185	-0.677264047	0.357587028
C	-3.686205266	-1.480371105	0.215045013
C	-4.791752346	-1.056202075	-0.530402040
C	-4.775587342	0.204121017	-1.113483078
C	-3.666294263	1.034645076	-0.966522068
C	-2.540399184	0.601802043	-0.241818016
C	0.014299999	1.057684078	-0.099181009
C	0.473343032	-0.136777010	-0.582241043
C	1.027903073	1.986175145	0.420148029
C	1.876690135	-0.546282041	-0.521822040
C	2.391464174	1.572331115	0.465982034
C	2.800734203	0.278391022	-0.016658002
H	-1.760024125	-1.017230075	0.950356068
H	-3.705374267	-2.446902174	0.685069051
H	-5.645596406	-1.698304124	-0.638779044
H	-5.619182402	0.543788039	-1.685645120
H	-3.669376265	2.007696144	-1.415141103
C	-1.395328098	1.486001106	-0.122798010

O	-1.648808118	2.801483200	-0.392017030
H	2.125831155	-1.522266110	-0.889516062
H	3.125200223	2.246220164	0.862361062
O	4.116996298	0.051418005	0.110535009
C	4.634779335	-1.181500087	-0.310141022
H	5.693939410	-1.147019083	-0.107802010
H	4.474397321	-1.330613097	-1.372365097
H	4.188512302	-2.001101145	0.242300017
H	-0.215180017	-0.832632059	-1.018410072
O	0.729334051	3.147581224	0.775863056
H	-0.905376065	3.326564242	-0.118039007
C	3.549378254	5.314844380	1.678657122
O	2.272342163	5.796573417	1.393270102
H	1.695510121	5.065621364	1.216061087
H	3.549467256	4.621271334	2.517424181
H	4.166079298	6.163114441	1.942656138
H	4.003631286	4.819681348	0.821689059
C	-4.523987325	5.497578396	-0.378054027
O	-4.554915327	4.117455296	-0.165418014
H	-3.670691265	3.775275269	-0.151773009
H	-5.548209398	5.845662422	-0.394359026
H	-4.059840292	5.757897413	-1.327310094
H	-4.000469288	6.024234433	0.416725030

Coord_7

C	-2.570221185	-0.672609049	0.353816026
C	-3.661055265	-1.484933105	0.234596017
C	-4.784813346	-1.074781075	-0.494752036
C	-4.790513347	0.182722015	-1.083133080
C	-3.687213264	1.025529072	-0.958792069
C	-2.543243184	0.606782045	-0.252395021
C	0.012406000	1.057603077	-0.117116006
C	0.478325035	-0.116275011	-0.630782043
C	1.010952075	1.970090141	0.451710034
C	1.880805133	-0.530047036	-0.553240039
C	2.372883173	1.555888112	0.515762040
C	2.792652200	0.277489019	-0.000707002
H	-1.726982123	-1.003475071	0.931298067
H	-3.663128264	-2.449736178	0.708440053
H	-5.633555407	-1.726193125	-0.586411044
H	-5.646725406	0.510928037	-1.643148117
H	-3.707299266	1.995630146	-1.412974101
C	-1.403451101	1.492802108	-0.158962009
O	-1.637373116	2.792482202	-0.514437038
H	2.138060155	-1.494190109	-0.945593071
H	3.098184221	2.215024160	0.950641067
O	4.105461298	0.045813002	0.147963012

C	4.632445335	-1.174121086	-0.298963021
H	5.686870411	-1.146695083	-0.072247003
H	4.495544323	-1.290130095	-1.368539098
H	4.173816298	-2.009847143	0.217974014
H	-0.202955017	-0.798627060	-1.099375080
O	0.699168053	3.121972225	0.827480058
H	-0.913359064	3.330374238	-0.214219015
C	3.535802254	5.301090381	1.670501120
O	2.238476163	5.769928416	1.467198105
H	1.660656121	5.034173360	1.313893096
H	3.596284261	4.606904330	2.506702183
H	4.159112299	6.155555440	1.896236138
H	3.939994282	4.811428347	0.785761057
C	-4.497539321	5.525432398	-0.384802027
O	-4.523079326	4.150252300	-0.141433008
H	-3.643761260	3.798650272	-0.190255012
H	-5.516922397	5.883148423	-0.326751023
H	-4.108659296	5.761726412	-1.373311097
H	-3.907829280	6.062890435	0.354402027

Coord_8

C	-2.548617185	-0.671693048	0.351860023
C	-3.629779260	-1.497074109	0.258567016
C	-4.773240345	-1.106739079	-0.454398032
C	-4.805727346	0.146211012	-1.050644073
C	-3.711913268	1.005293070	-0.951762071
C	-2.548366186	0.606544042	-0.264021018
C	0.006128000	1.055506074	-0.136521010
C	0.479971036	-0.095646004	-0.682330051
C	0.988528073	1.949598139	0.482287033
C	1.881321134	-0.514062036	-0.588772042
C	2.348500167	1.534539112	0.563556043
C	2.779769200	0.273900022	0.011661003
H	-1.690017124	-0.989043074	0.913938063
H	-3.611015259	-2.458779176	0.738208052
H	-5.614247406	-1.770454129	-0.527230035
H	-5.675759409	0.458521032	-1.598348114
H	-3.752878271	1.971002141	-1.413487101
C	-1.415984104	1.496022110	-0.197099014
O	-1.632020118	2.773052200	-0.639597046
H	2.147406155	-1.464752105	-1.007056071
H	3.064441218	2.176953159	1.037267076
O	4.088726295	0.036842003	0.181011015
C	4.625701331	-1.168326082	-0.293820021
H	5.674871407	-1.148943081	-0.043126004
H	4.512360327	-1.249075090	-1.369339098
H	4.155718299	-2.020051147	0.185339013

H	-0.193275016	-0.762802056	-1.184096088
O	0.663010049	3.090724224	0.879488063
H	-0.935204067	3.331094242	-0.312667023
C	3.504699253	5.301343380	1.668337118
O	2.187797159	5.742616414	1.545566113
H	1.618191118	4.995953359	1.414961103
H	3.631216262	4.608529333	2.498400180
H	4.122278297	6.168920442	1.856747132
H	3.864231277	4.820588347	0.759766055
C	-4.438719317	5.571174400	-0.391899029
O	-4.472282321	4.203036302	-0.112343007
H	-3.607890261	3.829529278	-0.224691015
H	-5.442060390	5.953057426	-0.257889018
H	-4.129755296	5.775098414	-1.415175103
H	-3.777893273	6.112439438	0.281386023

Coord_9

C	-2.524247181	-0.675201049	0.352493025
C	-3.591977261	-1.517544108	0.288208022
C	-4.756888345	-1.153168085	-0.407200030
C	-4.821805349	0.093257007	-1.013502075
C	-3.741458271	0.972669070	-0.943432069
C	-2.556605185	0.600166044	-0.275599020
C	-0.005415002	1.050879076	-0.157285009
C	0.477578033	-0.074903008	-0.737040052
C	0.959745069	1.924223137	0.511560039
C	1.877779134	-0.497845035	-0.629368044
C	2.317662167	1.508282109	0.608286046
C	2.761649198	0.268108018	0.019055001
H	-1.648949117	-0.974383070	0.898394064
H	-3.548068255	-2.474603180	0.775344055
H	-5.587158400	-1.832230133	-0.458709033
H	-5.707054412	0.384989027	-1.548044112
H	-3.807732276	1.932338139	-1.414376103
C	-1.433942104	1.494811109	-0.236519015
O	-1.633913117	2.742240198	-0.765900056
H	2.153576156	-1.433124102	-1.075062079
H	3.023335216	2.132014151	1.120808082
O	4.066563294	0.025399000	0.207568014
C	4.614559334	-1.162742082	-0.297209020
H	5.658095409	-1.152127083	-0.023502000
H	4.524313325	-1.205898085	-1.377032097
H	4.134821295	-2.030411146	0.141913008
H	-0.186839014	-0.725167050	-1.272417094
O	0.619722043	3.053032220	0.931888068
H	-0.973608069	3.328122240	-0.412663029
C	3.453375251	5.315658382	1.675145121

O	2.117901153	5.713610410	1.630749118
H	1.566482113	4.950188359	1.519160110
H	3.650931263	4.626290331	2.494271179
H	4.051994292	6.202912444	1.830188134
H	3.774869274	4.848338349	0.745555053
C	-4.342271313	5.635944404	-0.403140029
O	-4.397588317	4.278249306	-0.079413005
H	-3.559955258	3.869552276	-0.254611019
H	-5.316263385	6.057722437	-0.193511013
H	-4.118726295	5.799749417	-1.455404104
H	-3.606268259	6.171250446	0.192387014

Coord_10

C	-2.587998186	-0.590960042	0.332717026
C	-3.639730263	-1.452526105	0.343815026
C	-4.823980347	-1.156304085	-0.355040024
C	-4.921975353	0.045266002	-1.041327077
C	-3.857878277	0.947642066	-1.048952077
C	-2.653758191	0.641994044	-0.379545026
C	-0.107633007	1.098730077	-0.285974021
C	0.386298026	-0.031917003	-0.837489059
C	0.837778059	1.985693144	0.388810026
C	1.784094128	-0.454196034	-0.688140052
C	2.192360160	1.573430115	0.527966036
C	2.650684189	0.323067023	-0.030117001
H	-1.697698121	-0.839067060	0.879797066
H	-3.570290259	-2.374280169	0.892125065
H	-5.641459404	-1.852586132	-0.347591023
H	-5.820845417	0.283978023	-1.579468112
H	-3.950017286	1.871328135	-1.582938113
C	-1.541429111	1.540555111	-0.414681030
O	-1.721796123	2.715771197	-1.097087076
H	2.070795149	-1.397205101	-1.109886080
H	2.885694208	2.204798159	1.047951074
O	3.950085285	0.084116005	0.195062015
C	4.510251323	-1.113295082	-0.273703020
H	5.546573399	-1.097543079	0.025960002
H	4.447123319	-1.176253083	-1.354439096
H	4.019093290	-1.972554144	0.169211014
H	-0.267275019	-0.692901049	-1.373826097
O	0.482637036	3.123937225	0.770030057
H	-1.109442079	3.355967240	-0.751548054
C	3.295239234	5.489293396	1.362540096
O	1.943695140	5.831201421	1.368208098
H	1.419580101	5.042773364	1.310497096
H	3.562500257	4.850640350	2.202868159
H	3.862678279	6.406412460	1.443278103

H	3.589487260	4.988850361	0.441203034
C	-4.275253306	5.761686417	-0.811152061
O	-4.370696313	4.443316317	-0.359280025
H	-3.573729255	3.971995287	-0.564273041
H	-5.204299374	6.256419450	-0.560900039
H	-4.137820296	5.818736418	-1.889043137
H	-3.463238247	6.303387455	-0.331540024

Coord_11

C	-2.611579187	-0.592189041	0.336549026
C	-3.676721266	-1.441516102	0.323181024
C	-4.841595350	-1.124817081	-0.393568028
C	-4.911619354	0.081883004	-1.075412077
C	-3.835392276	0.968620070	-1.058799076
C	-2.649933192	0.642376047	-0.368614029
C	-0.101462006	1.096491080	-0.273698019
C	0.392771028	-0.057768005	-0.796980059
C	0.850429062	2.013057143	0.354821024
C	1.782019129	-0.459385035	-0.662192047
C	2.212512161	1.610733116	0.482461037
C	2.663798191	0.353198027	-0.039131001
H	-1.735218127	-0.853865063	0.899702063
H	-3.629241261	-2.367010168	0.867535061
H	-5.669277406	-1.808964131	-0.404023030
H	-5.797855417	0.336548025	-1.626937116
H	-3.905542282	1.897636134	-1.587219114
C	-1.524986108	1.535531113	-0.378495027
O	-1.718590123	2.751796198	-0.970788072
H	2.073475151	-1.410607102	-1.061575076
H	2.910159210	2.264319164	0.968177070
O	3.968329284	0.118495010	0.163036013
C	4.521409327	-1.092893077	-0.277184022
H	5.562937401	-1.065709077	0.003043002
H	4.440095321	-1.191469088	-1.354029095
H	4.041360290	-1.938726139	0.202210015
H	-0.266976018	-0.736319053	-1.302413093
O	0.496935035	3.156924229	0.713071053
H	-1.080094078	3.381214244	-0.651079049
C	3.317040236	5.448778390	1.358767099
O	1.982724142	5.845184422	1.283266090
H	1.430466103	5.078084367	1.202449087
H	3.506024254	4.797946345	2.210785159
H	3.915454280	6.341754457	1.478118106
H	3.646800262	4.938421357	0.455067034
C	-4.325042313	5.734516414	-0.813923060
O	-4.437506321	4.414060319	-0.371919026
H	-3.622891261	3.952172286	-0.521417039

H	-5.273900380	6.219326448	-0.626738044
H	-4.114880299	5.795489418	-1.879791135
H	-3.553116256	6.282935453	-0.278993020

Coord_12

C	-2.634034188	-0.594066043	0.344789024
C	-3.711690267	-1.431291101	0.308918020
C	-4.857213350	-1.096071077	-0.425068028
C	-4.900173351	0.114156011	-1.104056081
C	-3.812780273	0.985436069	-1.065358074
C	-2.646027191	0.640428045	-0.355125026
C	-0.096479009	1.092918080	-0.259802020
C	0.396866030	-0.084714007	-0.754926052
C	0.862860060	2.036300148	0.320171021
C	1.776797128	-0.467971031	-0.637170043
C	2.231863162	1.641873117	0.433852032
C	2.674707191	0.378003025	-0.051968005
H	-1.771641127	-0.867823060	0.923666066
H	-3.685458263	-2.359223171	0.850569061
H	-5.694375409	-1.768201126	-0.451805032
H	-5.773810418	0.383356029	-1.668538121
H	-3.861686278	1.918490137	-1.589408114
C	-1.509263109	1.528314109	-0.341496023
O	-1.716834123	2.778388201	-0.841607058
H	2.071791150	-1.426898104	-1.014871072
H	2.934506211	2.315573166	0.883641062
O	3.983729284	0.145098010	0.125474011
C	4.528392323	-1.079917079	-0.286429018
H	5.575114399	-1.043119078	-0.027395003
H	4.427554318	-1.213760087	-1.357797096
H	4.059802292	-1.910663139	0.229271017
H	-0.269870020	-0.779095059	-1.228110088
O	0.512447035	3.185563228	0.655924048
H	-1.054488075	3.396924247	-0.547327039
C	3.327105241	5.426904388	1.363050096
O	2.011714144	5.859430424	1.203297088
H	1.443760104	5.107337370	1.093470081
H	3.442285246	4.766569341	2.220784159
H	3.940310286	6.302591456	1.527488111
H	3.701718266	4.912395356	0.479408033
C	-4.358927315	5.709480409	-0.811056057
O	-4.492804323	4.381999316	-0.396677029
H	-3.661923264	3.932347285	-0.478561032
H	-5.326403384	6.180957446	-0.701489051
H	-4.057329293	5.786869417	-1.853638131
H	-3.643420264	6.259303450	-0.204034015

Coord_13

C	-2.654551189	-0.597220045	0.355822026
C	-3.743648271	-1.422881104	0.298752022
C	-4.869575349	-1.071431076	-0.452570031
C	-4.886298350	0.140774013	-1.130345083
C	-3.788883274	0.997179073	-1.071047079
C	-2.641115188	0.635580046	-0.340757027
C	-0.091973006	1.087932077	-0.244658015
C	0.399229028	-0.112914010	-0.711719052
C	0.875679061	2.054864146	0.285303019
C	1.768877128	-0.480571033	-0.612652044
C	2.250799161	1.665765121	0.383291030
C	2.683747194	0.396345028	-0.067511005
H	-1.806384132	-0.881291066	0.950644067
H	-3.738030271	-2.351987170	0.839012063
H	-5.715352414	-1.731966126	-0.494487034
H	-5.747165412	0.422837033	-1.707927123
H	-3.817229272	1.933029139	-1.591990113
C	-1.493549106	1.518750108	-0.304609025
O	-1.716004124	2.795409203	-0.710641050
H	2.066128150	-1.446755104	-0.969432072
H	2.959026215	2.357125169	0.796094058
O	3.996376287	0.162336012	0.084244007
C	4.531184326	-1.076013079	-0.299533024
H	5.582912403	-1.031828075	-0.062822002
H	4.409981315	-1.244405091	-1.363887096
H	4.074000292	-1.890053136	0.251780016
H	-0.275209021	-0.821047062	-1.151871082
O	0.529904037	3.209336230	0.599086046
H	-1.031873077	3.402985247	-0.441310034
C	3.327415238	5.424063389	1.372191098
O	2.031602144	5.874277423	1.125916081
H	1.460394103	5.129670369	0.985031069
H	3.375324242	4.757457343	2.231348161
H	3.939251286	6.290662452	1.583580116
H	3.754994271	4.909392354	0.513018039
C	-4.378436313	5.686439407	-0.802545056
O	-4.532981327	4.348850315	-0.429675030
H	-3.691076263	3.912523284	-0.435705031
H	-5.358796387	6.143174444	-0.780470057
H	-3.975969286	5.789482415	-1.808178128
H	-3.734815271	6.232223450	-0.116582008

Coord_14

C	-2.672414192	-0.601910042	0.367868026
C	-3.771589269	-1.417032102	0.290160020
C	-4.877414353	-1.051978076	-0.479252032

C	-4.868765348	0.160794010	-1.157331086
C	-3.762756269	1.003389074	-1.078153077
C	-2.634482190	0.627718043	-0.327157024
C	-0.087511005	1.082129077	-0.228600015
C	0.400105028	-0.141878009	-0.667792049
C	0.889371062	2.068863149	0.250752021
C	1.758346125	-0.497135037	-0.588304043
C	2.269587166	1.681976122	0.332005023
C	2.691026191	0.407734028	-0.084644007
H	-1.838950134	-0.894257062	0.979345070
H	-3.785944271	-2.346157171	0.830244062
H	-5.730723415	-1.701710121	-0.535839040
H	-5.716496410	0.453795034	-1.748647127
H	-3.771261269	1.940905138	-1.597174113
C	-1.477470108	1.507234111	-0.268648017
O	-1.716233126	2.803126200	-0.578846043
H	2.056430146	-1.470202107	-0.925041064
H	2.984010213	2.388187170	0.707398050
O	4.006166289	0.169262010	0.041186003
C	4.529478327	-1.082190075	-0.314702022
H	5.585893401	-1.033266072	-0.100815008
H	4.387493314	-1.283981093	-1.370638101
H	4.083180295	-1.878007135	0.271030019
H	-0.282747019	-0.861333061	-1.074727078
O	0.549994039	3.228404233	0.543203039
H	-1.012227075	3.399813242	-0.334100025
C	3.320203240	5.439712393	1.383120101
O	2.044367148	5.889866424	1.048864074
H	1.481401106	5.144912368	0.878805065
H	3.308696238	4.770699342	2.241551159
H	3.915748280	6.305839456	1.638680120
H	3.806602276	4.927309354	0.554406039
C	-4.385848314	5.665123407	-0.788549059
O	-4.556490328	4.316472308	-0.465591036
H	-3.711320267	3.892698282	-0.392848029
H	-5.370374388	6.107898441	-0.857501061
H	-3.883068278	5.798925419	-1.744150125
H	-3.825473277	6.201794446	-0.026587003

Coord_15

C	-2.687078196	-0.607951045	0.379132030
C	-3.794556271	-1.414167099	0.280555019
C	-4.879544350	-1.038497074	-0.508230037
C	-4.846574347	0.173647011	-1.187852087
C	-3.733805267	1.004097071	-1.088707078
C	-2.625739187	0.617255045	-0.315825021
C	-0.083083008	1.076918078	-0.211882015

C	0.399167030	-0.170352010	-0.623563044
C	0.904164064	2.079224149	0.217137015
C	1.744755123	-0.516848038	-0.563856039
C	2.288257163	1.690851123	0.281252019
C	2.696270195	0.412431032	-0.102284009
H	-1.868999136	-0.906246064	1.008367071
H	-3.828116274	-2.342325166	0.821465059
H	-5.738991412	-1.678680120	-0.579605041
H	-5.680637407	0.475379037	-1.793945128
H	-3.723343269	1.942318141	-1.606793116
C	-1.461127103	1.494813109	-0.234256015
O	-1.718497126	2.802271203	-0.447043034
H	2.042008145	-1.496514107	-0.881571064
H	3.009628218	2.408751172	0.619449046
O	4.012649287	0.165672014	-0.001954998
C	4.522487324	-1.098735077	-0.330310026
H	5.583189401	-1.048155077	-0.139154010
H	4.359618315	-1.332309094	-1.376629102
H	4.086050293	-1.874955137	0.288200021
H	-0.292924024	-0.898345067	-0.997706070
O	0.573260042	3.243751235	0.489053035
H	-0.996499070	3.388474244	-0.226851016
C	3.307924238	5.472514392	1.392979102
O	2.052955150	5.906274427	0.970214069
H	1.507836108	5.153728371	0.776573058
H	3.245096235	4.805825344	2.250888164
H	3.874683279	6.346272456	1.685602124
H	3.856073279	4.963282358	0.601680041
C	-4.384154317	5.645236407	-0.769467054
O	-4.564842327	4.286387306	-0.498572034
H	-3.724554270	3.872874276	-0.349992027
H	-5.363628384	6.076640439	-0.926041067
H	-3.790266273	5.810486418	-1.666028122
H	-3.911401280	6.168965443	0.058047003

Coord_16

C	-2.698113193	-0.614626045	0.388031029
C	-3.811551274	-1.414331102	0.267573020
C	-4.874798349	-1.031478072	-0.542271042
C	-4.818948348	0.179130013	-1.224296091
C	-3.701811264	0.999857070	-1.104308081
C	-2.614819191	0.605214045	-0.307951022
C	-0.079153005	1.074690078	-0.194582015
C	0.395407030	-0.196185014	-0.579329044
C	0.920022067	2.087817151	0.185189013
C	1.726979123	-0.538040037	-0.539035038
C	2.306545164	1.693583122	0.232300017

C	2.698730192	0.411511031	-0.119369010
H	-1.896269137	-0.916190067	1.036420075
H	-3.863266280	-2.340771168	0.810015060
H	-5.738562414	-1.663954118	-0.629168047
H	-5.638691405	0.487035033	-1.846528132
H	-3.673578266	1.938044141	-1.622170118
C	-1.445133102	1.483318109	-0.201791012
O	-1.724705126	2.794127203	-0.315881024
H	2.021360146	-1.524148108	-0.838905058
H	3.035918220	2.419631173	0.534105038
O	4.014895290	0.152113011	-0.043569004
C	4.508761324	-1.125222081	-0.344931024
H	5.573318404	-1.076555079	-0.175894014
H	4.325071312	-1.388482101	-1.380693098
H	4.080621295	-1.880624134	0.304360020
H	-0.307006023	-0.929544067	-0.921668068
O	0.600131044	3.257331236	0.437556029
H	-0.986754070	3.370844243	-0.120776007
C	3.293528235	5.520428397	1.399244100
O	2.061373148	5.923676426	0.888570063
H	1.540878110	5.157718372	0.680161049
H	3.186439228	4.861995350	2.259042161
H	3.822597273	6.408580463	1.718158124
H	3.903161281	5.013538363	0.652657045
C	-4.377030316	5.626515407	-0.745948052
O	-4.562587329	4.259385307	-0.524030037
H	-3.733752270	3.853049275	-0.307136021
H	-5.344025383	6.050091436	-0.981305068
H	-3.706217268	5.820317420	-1.580364115
H	-3.988889286	6.135319443	0.133244011

Coord_17

C	-2.704969197	-0.620541045	0.393497028
C	-3.821233276	-1.417142102	0.249447017
C	-4.861746351	-1.031153073	-0.583429040
C	-4.785149347	0.177365011	-1.268304090
C	-3.666808263	0.991786069	-1.125886082
C	-2.601827185	0.593356040	-0.304165024
C	-0.076605006	1.079079079	-0.176437014
C	0.387055030	-0.216114015	-0.535100039
C	0.936764066	2.097611153	0.155832010
C	1.703093120	-0.558079042	-0.513466035
C	2.323967166	1.692259121	0.186437014
C	2.697130193	0.406872030	-0.134851011
H	-1.920318137	-0.922225069	1.062637077
H	-3.889541280	-2.341393169	0.793801058
H	-5.727416411	-1.658539121	-0.687137049

H	-5.589866401	0.488393035	-1.908264136
H	-3.622555260	1.929464140	-1.643925119
C	-1.430542103	1.475568107	-0.171147014
O	-1.737705128	2.780676199	-0.185754015
H	1.991956142	-1.550648114	-0.796835059
H	3.062895221	2.422434172	0.453133034
O	4.011398290	0.129794008	-0.082242008
C	4.485967321	-1.160640084	-0.357383025
H	5.553943399	-1.118084078	-0.209479016
H	4.281457306	-1.450991105	-1.381935098
H	4.063992291	-1.894092134	0.320454025
H	-0.327215022	-0.951182066	-0.847090059
O	0.631165046	3.272239233	0.389845028
H	-0.986254071	3.349846241	-0.017088001
C	3.281148234	5.580719403	1.399982101
O	2.075084152	5.942512427	0.803307056
H	1.582201112	5.159491370	0.591413044
H	3.134508228	4.938006355	2.265724161
H	3.768338269	6.488010465	1.731706126
H	3.948803284	5.073136364	0.705262053
C	-4.368912313	5.608752403	-0.718820050
O	-4.556127329	4.235407307	-0.540445041
H	-3.743066271	3.833225274	-0.264280019
H	-5.318596384	6.027998434	-1.022329074
H	-3.635525262	5.826594420	-1.492420106
H	-4.058181290	6.102187439	0.199018012

Coord_18

C	-2.706493196	-0.623340044	0.395411030
C	-3.821293274	-1.421663102	0.225492014
C	-4.838128350	-1.037541073	-0.632565048
C	-4.744106344	0.168739014	-1.320369093
C	-3.628858259	0.981673069	-1.153369083
C	-2.586756186	0.584471043	-0.304199023
C	-0.076662003	1.095554076	-0.156601011
C	0.371385028	-0.225262018	-0.490381037
C	0.954320071	2.113031151	0.130313009
C	1.670072121	-0.573093039	-0.486559033
C	2.339933168	1.689932122	0.144973013
C	2.689541193	0.401291031	-0.147690010
H	-1.940011140	-0.921273068	1.087016077
H	-3.903736280	-2.343590170	0.771843055
H	-5.702425413	-1.663550117	-0.754818052
H	-5.533152401	0.479075033	-1.979806143
H	-3.571288256	1.918667136	-1.671717121
C	-1.418737101	1.475832108	-0.141480009
O	-1.761345126	2.764939198	-0.056627003

H	1.949737138	-1.572404115	-0.754966053
H	3.090799224	2.419463175	0.378134028
O	3.999832286	0.100389009	-0.116867007
C	4.450403318	-1.203627089	-0.366864024
H	5.521365395	-1.172357084	-0.238968016
H	4.224640301	-1.517911108	-1.379818098
H	4.031825289	-1.913932137	0.337195024
H	-0.357054025	-0.957632070	-0.773765053
O	0.667536049	3.293091235	0.347413024
H	-0.999682071	3.329961242	0.083172005
C	3.277292236	5.649891405	1.394275099
O	2.101896150	5.963683427	0.714893052
H	1.634787117	5.162801374	0.512241037
H	3.092310221	5.032128360	2.270682166
H	3.724300270	6.578479475	1.723848124
H	3.996380288	5.135680368	0.758183053
C	-4.365472312	5.591733401	-0.689012051
O	-4.552079329	4.213609305	-0.550743042
H	-3.758080268	3.813400273	-0.221424017
H	-5.294219379	6.009151432	-1.053527073
H	-3.579296258	5.830471421	-1.402222103
H	-4.127625294	6.069428435	0.258428017

Coord_19

C	-2.611519188	-0.702909050	0.416026030
C	-3.722309267	-1.494049109	0.177638013
C	-4.717291340	-1.066234074	-0.680956047
C	-4.610116330	0.174598012	-1.303421096
C	-3.500459252	0.977342070	-1.068714079
C	-2.479381179	0.536197039	-0.217655016
C	0.011367002	1.067394078	-0.025149001
C	0.430194031	-0.263202021	-0.412811029
C	1.069974077	2.056642150	0.269899019
C	1.707696121	-0.627418047	-0.452347031
C	2.449073177	1.602946114	0.237246015
C	2.762397200	0.326607023	-0.102378007
H	-1.861971133	-1.034032072	1.111184078
H	-3.815631273	-2.442894175	0.673873047
H	-5.578295400	-1.684541124	-0.855018061
H	-5.384957386	0.519255038	-1.962581143
H	-3.432964249	1.941186141	-1.534327113
C	-1.317771092	1.427928105	0.023350999
O	-1.702131123	2.677761194	0.278511019
H	1.967895141	-1.619117115	-0.764833054
H	3.219111229	2.310687166	0.475157036
O	4.064676295	-0.010627001	-0.116938007
C	4.478374320	-1.315829096	-0.418769030

H	5.552343400	-1.312456094	-0.314319025
H	4.224321303	-1.592607112	-1.435949104
H	4.060354293	-2.039750145	0.271593021
H	-0.319766021	-0.969083069	-0.706132052
O	0.813908058	3.230410232	0.539201041
H	-0.932742065	3.234980234	0.413852032
C	3.407998244	5.554712399	1.730660122
O	2.266502163	5.865824420	0.994396072
H	1.813629130	5.062804363	0.770384055
H	3.183386230	4.924698356	2.588815188
H	3.828472278	6.483168467	2.094007149
H	4.164198300	5.054511362	1.127197082
C	-4.269606307	5.545711401	-0.280331018
O	-4.454673318	4.160483302	-0.263649017
H	-3.685316264	3.738294267	0.095327006
H	-5.171266374	5.988058432	-0.681470048
H	-3.433295245	5.840904420	-0.910528066
H	-4.108574294	5.948627430	0.716704050

LIIC path connecting S1-PP-KETO and S0-KETO

Coord_1

C	-2.635786188	-0.672508050	0.206697014
C	-3.774533273	-1.510265111	0.024553004
C	-4.920704354	-1.053976075	-0.558274039
C	-4.997388361	0.296223020	-0.945500068
C	-3.877278280	1.194591086	-0.770671054
C	-2.598325186	0.699614049	-0.306705022
C	-0.117274008	1.148232084	-0.142768011
C	0.331478026	-0.191503013	-0.389666028
C	0.924319066	2.154810155	0.134237012
C	1.644304121	-0.562960041	-0.305476023
C	2.298672165	1.703757121	0.264803021
C	2.648913192	0.410289029	0.047887001
H	-1.836832134	-1.028998073	0.823261060
H	-3.720110266	-2.520688184	0.384840027
H	-5.765215415	-1.701971121	-0.691515049
H	-5.896692424	0.685371047	-1.380154099
H	-4.007025286	2.229213159	-1.000284074
C	-1.479189108	1.544761112	-0.260761017
O	-1.784070130	2.865855205	-0.394693027
H	1.919123138	-1.571076113	-0.542699040
H	3.038310218	2.443452177	0.503044037
O	3.955194285	0.093156008	0.164223010
C	4.399741317	-1.216021087	-0.054307006
H	5.462319396	-1.201911089	0.135099010
H	4.228593303	-1.533498109	-1.077625075
H	3.932161284	-1.920182139	0.625678044

H	-0.372779024	-0.925755067	-0.720476052
O	0.658249046	3.346554240	0.262067021
H	-0.987026072	3.376814241	-0.237622016
C	2.656111193	6.005083435	1.829757129
O	2.923659210	5.194923375	0.727122053
H	2.142245153	4.699605336	0.505378037
H	1.914941135	6.770430490	1.605878116
H	3.577790257	6.499892468	2.107922151
H	2.305170166	5.431832388	2.685268193
C	-4.244869303	5.779828417	-0.693238050
O	-4.353598315	4.523321324	-0.089960005
H	-3.493088252	4.129923300	-0.009919999
H	-5.244085375	6.184853445	-0.781812056
H	-3.808767273	5.720562412	-1.687925122
H	-3.651505261	6.468444464	-0.096766008

Coord_2

C	-2.649780190	-0.648875047	0.258594020
C	-3.797312274	-1.477166106	0.132538009
C	-4.948778355	-1.025574074	-0.448588031
C	-5.012203360	0.306826023	-0.890629065
C	-3.884519282	1.191315087	-0.773722058
C	-2.611121189	0.698951048	-0.299535019
C	-0.108661008	1.109955080	-0.183431012
C	0.359225027	-0.211934017	-0.446199034
C	0.902206066	2.123633153	0.136542007
C	1.684902123	-0.559285043	-0.349810027
C	2.280086164	1.707163123	0.277768022
C	2.659316192	0.421279029	0.033598003
H	-1.832895134	-0.996621072	0.857069062
H	-3.749069269	-2.474908176	0.527324039
H	-5.804016416	-1.666632120	-0.541931040
H	-5.913227424	0.689379052	-1.328114094
H	-4.004705288	2.214833159	-1.057385077
C	-1.473028104	1.526611111	-0.302948022
O	-1.733500126	2.843530206	-0.529960040
H	1.981363141	-1.559238111	-0.596165046
H	3.002480214	2.452502177	0.548724041
O	3.971378287	0.133666008	0.161943013
C	4.446183320	-1.162500084	-0.068947006
H	5.506200398	-1.128890079	0.131933011
H	4.292079306	-1.469518108	-1.098145082
H	3.985679287	-1.884990137	0.596509042
H	-0.329623021	-0.955697070	-0.789145055
O	0.588184042	3.310346240	0.288010020
H	-0.931977065	3.350815239	-0.394406027
C	2.680505195	5.886326424	1.928438140

O	2.808324203	5.277964382	0.680117048
H	2.029269144	4.762759344	0.501278035
H	1.864009132	6.605846475	1.952073143
H	3.602099257	6.415626463	2.133392155
H	2.519185183	5.161874372	2.723934195
C	-4.283685306	5.813735418	-0.777044058
O	-4.360604315	4.551282330	-0.181958015
H	-3.491350254	4.176977301	-0.101744005
H	-5.292666382	6.194970446	-0.859637064
H	-3.849745277	5.771345415	-1.773518129
H	-3.705061264	6.512423470	-0.177928013

Coord_3

C	-2.656300189	-0.621056046	0.302413024
C	-3.808518274	-1.441426104	0.227505015
C	-4.965901356	-0.997208072	-0.353136023
C	-5.021382363	0.316010021	-0.846199063
C	-3.890233280	1.187527088	-0.781729054
C	-2.621387190	0.702547051	-0.296465024
C	-0.102135009	1.079718077	-0.221170018
C	0.383714028	-0.223338014	-0.504799037
C	0.877549063	2.095295151	0.149810010
C	1.720680125	-0.549043039	-0.392412029
C	2.256702160	1.710166124	0.305623023
C	2.664395193	0.433986030	0.029315001
H	-1.822413133	-0.960051071	0.882882063
H	-3.763307269	-2.426101174	0.654106049
H	-5.828621417	-1.632684119	-0.409975031
H	-5.924967428	0.689492052	-1.286771095
H	-4.003875290	2.197489157	-1.115492078
C	-1.468596107	1.514982107	-0.344743023
O	-1.693400122	2.818286202	-0.664496047
H	2.038157147	-1.539421111	-0.651709045
H	2.961297211	2.457232174	0.615570044
O	3.980440289	0.173125015	0.173882014
C	4.484379323	-1.108689081	-0.073643005
H	5.540561401	-1.058485078	0.143271009
H	4.350703313	-1.399188102	-1.110460079
H	4.027888290	-1.851895132	0.571476043
H	-0.289338022	-0.973199068	-0.866453062
O	0.516203035	3.274207238	0.329032026
H	-0.890016066	3.324699241	-0.548735037
C	2.730501195	5.763481413	1.998407146
O	2.679368194	5.360657387	0.663934045
H	1.907359137	4.822983345	0.527904038
H	1.888162137	6.398075458	2.267521162
H	3.639792262	6.334216454	2.135325155

H	2.752596197	4.917626352	2.682303191
C	-4.337492313	5.842068420	-0.843704061
O	-4.378685317	4.570964331	-0.264149021
H	-3.500017251	4.218232304	-0.187024014
H	-5.356606387	6.197151445	-0.917227064
H	-3.907226283	5.823291417	-1.842477132
H	-3.774885271	6.548382472	-0.238421016

Coord_4

C	-2.656379190	-0.590748043	0.336630027
C	-3.810405272	-1.404033101	0.307407023
C	-4.973915360	-0.968317069	-0.273537017
C	-5.025061362	0.325325023	-0.812811058
C	-3.893268280	1.184149085	-0.794697056
C	-2.628526188	0.709434049	-0.298115020
C	-0.096215007	1.055320074	-0.256209018
C	0.406457029	-0.227701017	-0.565419043
C	0.851587061	2.066669149	0.173670015
C	1.752975124	-0.534910038	-0.432820030
C	2.229648158	1.708987123	0.348354023
C	2.665346193	0.444968030	0.035323005
H	-1.806672132	-0.921975064	0.899069066
H	-3.766317272	-2.375932171	0.762411053
H	-5.841788422	-1.599036113	-0.297705024
H	-5.931626425	0.688545047	-1.256368090
H	-4.001801291	2.179207157	-1.173788085
C	-1.464224108	1.508462109	-0.386314029
O	-1.660522117	2.790084198	-0.796378056
H	2.090781152	-1.514230109	-0.708646051
H	2.915681212	2.453106174	0.703467052
O	3.983435289	0.207417013	0.200722016
C	4.515291323	-1.058679074	-0.067371006
H	5.566264402	-0.995354073	0.170349015
H	4.405502316	-1.326361094	-1.113094080
H	4.059694292	-1.824678134	0.551198039
H	-0.250395016	-0.979797072	-0.952418071
O	0.443455033	3.234811230	0.384095030
H	-0.857296063	3.297666237	-0.698396052
C	2.793797202	5.645789408	2.034902146
O	2.537430182	5.440335394	0.678925049
H	1.778296129	4.876680352	0.584688043
H	1.975254144	6.161679445	2.533149181
H	3.678646265	6.264028453	2.111818149
H	2.982242216	4.713545341	2.563195182
C	-4.399340317	5.866756422	-0.888502063
O	-4.402570315	4.584395332	-0.333086026
H	-3.514471251	4.254608308	-0.262335017

H	-5.428287393	6.194568446	-0.949895070
H	-3.974557288	5.878538422	-1.889712134
H	-3.853000278	6.576784473	-0.272858019

Coord_5

C	-2.650597193	-0.559249043	0.360689028
C	-3.804640272	-1.365707100	0.371623026
C	-4.974168359	-0.938321069	-0.210050014
C	-5.023122361	0.336171024	-0.790259058
C	-3.892379279	1.182066084	-0.812323056
C	-2.631753191	0.718869052	-0.304666022
C	-0.089433008	1.034816075	-0.288974022
C	0.428885031	-0.226766014	-0.628061045
C	0.825582058	2.034818145	0.207015013
C	1.783004129	-0.519458036	-0.470926031
C	2.200045157	1.699925121	0.404891029
C	2.663288191	0.450829033	0.051055005
H	-1.786388127	-0.884451063	0.904978066
H	-3.760805272	-2.325654167	0.851286059
H	-5.845680420	-1.564652112	-0.205469016
H	-5.932761426	0.689016052	-1.236428088
H	-3.995830287	2.161854155	-1.231612088
C	-1.458215105	1.505889106	-0.427865032
O	-1.631753116	2.759052197	-0.924470066
H	2.140337152	-1.486198109	-0.766518055
H	2.866573208	2.435608177	0.810846059
O	3.981310288	0.232341018	0.241977018
C	4.539705329	-1.016691071	-0.050138004
H	5.583992401	-0.944371068	0.213062017
H	4.457169320	-1.255226088	-1.105375077
H	4.081961293	-1.806978128	0.535437040
H	-0.211374015	-0.976722070	-1.046754075
O	0.371183026	3.189094232	0.451191033
H	-0.830185058	3.269225235	-0.842240060
C	2.857767207	5.542145397	2.035772145
O	2.383265170	5.514012398	0.723704055
H	1.643871116	4.920282356	0.669278048
H	2.110064154	5.912992427	2.734034199
H	3.706653267	6.212630445	2.062862147
H	3.186539232	4.561989327	2.374757170
C	-4.462495320	5.889459423	-0.908190066
O	-4.427066321	4.593597332	-0.386351029
H	-3.530025253	4.287181310	-0.325186024
H	-5.500473398	6.189959444	-0.954495070
H	-4.045337290	5.938613427	-1.911456138
H	-3.931567283	6.598112475	-0.277754020

Coord_6

C	-2.639162191	-0.527422037	0.374845027
C	-3.792363270	-1.326778096	0.420739030
C	-4.967585357	-0.906489063	-0.161776010
C	-5.015279362	0.349869025	-0.777658057
C	-3.886313277	1.182130083	-0.834051058
C	-2.630163188	0.730334053	-0.315932021
C	-0.080396005	1.016539071	-0.320020021
C	0.452338035	-0.222051018	-0.692670047
C	0.800743060	1.997159145	0.248086020
C	1.811878130	-0.505076035	-0.506848038
C	2.168954158	1.679612123	0.473226037
C	2.659247193	0.448424033	0.075249005
H	-1.761814125	-0.848890061	0.900760063
H	-3.748760271	-2.275958163	0.921325065
H	-5.841926420	-1.528374112	-0.132151011
H	-5.927847427	0.693110048	-1.225863090
H	-3.983524286	2.147055152	-1.288446095
C	-1.448915105	1.506318110	-0.469650031
O	-1.604324118	2.725324196	-1.048382073
H	2.187797159	-1.457725102	-0.824933059
H	2.814876200	2.400614172	0.934810068
O	3.974909286	0.243917019	0.296169023
C	4.558283329	-0.986791070	-0.022772000
H	5.594298403	-0.910261065	0.270191019
H	4.506146326	-1.190113087	-1.087278078
H	4.095534293	-1.802036131	0.523352039
H	-0.170956013	-0.964990068	-1.148764082
O	0.300633020	3.134474223	0.527425037
H	-0.805470057	3.239001235	-0.980132073
C	2.909993207	5.460587393	2.001332142
O	2.217638158	5.578643403	0.795107057
H	1.505771110	4.950582358	0.777581056
H	2.275370163	5.669488410	2.860128205
H	3.712378267	6.186357446	1.990045146
H	3.346193241	4.472127320	2.129456151
C	-4.520595325	5.911424427	-0.900945063
O	-4.447254322	4.600434329	-0.422541032
H	-3.542143253	4.317030310	-0.374059025
H	-5.566448402	6.185487447	-0.929313065
H	-4.113519297	6.004307433	-1.905249138
H	-4.003076290	6.612711475	-0.251499018

Coord_7

C	-2.621997189	-0.495663036	0.380016026
C	-3.774274272	-1.287122093	0.456334032
C	-4.954725355	-0.871877060	-0.126874008

C	-5.001125357	0.367689027	-0.773575057
C	-3.873882279	1.185134085	-0.859123063
C	-2.622802189	0.743543053	-0.331420023
C	-0.067833004	0.999135071	-0.349944026
C	0.478049032	-0.214837015	-0.759035055
C	0.778168057	1.951654140	0.294633023
C	1.840594134	-0.493866034	-0.540794039
C	2.137338156	1.645317119	0.550609039
C	2.654146189	0.435108029	0.106140007
H	-1.732867125	-0.816058058	0.887216062
H	-3.731543267	-2.226883159	0.974394071
H	-5.831688418	-1.488830109	-0.075444007
H	-5.916330424	0.702783053	-1.223097086
H	-3.962730287	2.136115153	-1.343892096
C	-1.434786105	1.509017110	-0.511964039
O	-1.575976114	2.688900195	-1.168370083
H	2.234034159	-1.430998100	-0.883442065
H	2.761404199	2.344816167	1.071371078
O	3.964973285	0.238731019	0.361063024
C	4.571593327	-0.972565071	0.013298002
H	5.597646402	-0.897181062	0.339669023
H	4.552712325	-1.135208079	-1.059275076
H	4.101244295	-1.812417129	0.513763035
H	-0.127912010	-0.945488066	-1.257282090
O	0.232977015	3.069111223	0.609195046
H	-0.780528055	3.206599230	-1.112831079
C	2.938699210	5.407625387	1.933997141
O	2.041283145	5.631454404	0.888259065
H	1.365509098	4.965134356	0.903929067
H	2.452847179	5.448697394	2.906595212
H	3.685241264	6.189757447	1.896102134
H	3.444681250	4.448755323	1.842739133
C	-4.567747331	5.933408429	-0.866302062
O	-4.458635321	4.606495329	-0.441209030
H	-3.546598253	4.345118313	-0.408406031
H	-5.620082406	6.182678447	-0.873933062
H	-4.173454298	6.075620439	-1.869930133
H	-4.060480290	6.620703475	-0.194283014

Coord_8

C	-2.598838186	-0.463935034	0.377627029
C	-3.750717270	-1.246174088	0.480732035
C	-4.935858355	-0.833335060	-0.102811006
C	-4.980183358	0.390836028	-0.776191056
C	-3.854004276	1.191789087	-0.886637063
C	-2.608721190	0.758416055	-0.350395028
C	-0.050642003	0.981615071	-0.379295027

C	0.507131037	-0.206144014	-0.826725059
C	0.758788056	1.897015134	0.344125023
C	1.870046134	-0.487504033	-0.572940043
C	2.106015149	1.595252115	0.633830046
C	2.648785189	0.409000027	0.141700009
H	-1.699252124	-0.786123056	0.865658064
H	-3.709999266	-2.177825158	1.013327070
H	-5.815718420	-1.444435101	-0.032161001
H	-5.897646425	0.719728050	-1.226221089
H	-3.931618285	2.129964156	-1.397653102
C	-1.414467101	1.513455108	-0.555121042
O	-1.545079111	2.649553189	-1.285168090
H	2.279848166	-1.407872102	-0.941443067
H	2.706830197	2.266140163	1.215817089
O	3.952136286	0.214312018	0.433953031
C	4.580136328	-0.976756070	0.056310005
H	5.594429401	-0.908259065	0.418905029
H	4.597048330	-1.094199081	-1.022178073
H	4.099918293	-1.839746133	0.505435034
H	-0.081101007	-0.919035067	-1.370677101
O	0.169245013	2.992144218	0.692474051
H	-0.753454056	3.171505227	-1.241802089
C	2.933080210	5.387510386	1.837727131
O	1.854861134	5.670327410	0.996791070
H	1.224362090	4.962659357	1.041406073
H	2.623808187	5.266698379	2.873690208
H	3.615721259	6.225033450	1.784352128
H	3.468593251	4.491288325	1.531401112
C	-4.598555332	5.955691427	-0.805034057
O	-4.457211321	4.613036330	-0.442754032
H	-3.539587253	4.372218316	-0.428572028
H	-5.655819407	6.182448445	-0.789073056
H	-4.219885305	6.151815443	-1.805589128
H	-4.097279297	6.622001478	-0.107926007

Coord_9

C	-2.569320187	-0.431840031	0.369428025
C	-3.721782270	-1.203010089	0.496711034
C	-4.911022352	-0.789574059	-0.086662009
C	-4.951936358	0.420407030	-0.783498057
C	-3.825737273	1.202688085	-0.915631065
C	-2.587040184	0.775042058	-0.371965028
C	-0.027924001	0.963406071	-0.408471029
C	0.540572039	-0.196699015	-0.895055066
C	0.743300054	1.832850133	0.394030026
C	1.901023139	-0.487106033	-0.603329042
C	2.075599147	1.528822108	0.719563052

C	2.643819189	0.369214026	0.179905014
H	-1.660592117	-0.758773054	0.837751060
H	-3.684577263	-2.127650154	1.041573076
H	-5.794427418	-1.393461103	0.001382999
H	-5.871227425	0.745351055	-1.233191089
H	-3.888689278	2.129123156	-1.449529105
C	-1.386824098	1.519297108	-0.599439044
O	-1.510707106	2.606777189	-1.399786099
H	2.326002170	-1.389727101	-0.998125073
H	2.651606191	2.164085156	1.363197096
O	3.936903284	0.169461013	0.512013036
C	4.584363332	-1.000923071	0.104448005
H	5.584992403	-0.945179069	0.505154036
H	4.639299334	-1.069878079	-0.976957073
H	4.092382296	-1.884492134	0.497345036
H	-0.029444004	-0.886419063	-1.486929109
O	0.110233008	2.903843210	0.773179058
H	-0.723151054	3.133033226	-1.368972097
C	2.883571207	5.401580389	1.717342122
O	1.658896120	5.694128411	1.113246080
H	1.083270079	4.943359358	1.182345083
H	2.769837199	5.136382369	2.766145199
H	3.495533252	6.291574451	1.658092120
H	3.407897245	4.593224331	1.211850085
C	-4.608124333	5.978160431	-0.718948053
O	-4.439522317	4.620972333	-0.428259031
H	-3.517808254	4.398888315	-0.435661030
H	-5.668631407	6.185216444	-0.676357047
H	-4.247913305	6.231576446	-1.713436122
H	-4.107555295	6.616377478	0.004396002

Coord_10

C	-2.361268172	-0.412923029	0.274232017
C	-3.525952255	-1.149798083	0.446358030
C	-4.719454341	-0.717282049	-0.123326007
C	-4.745104340	0.473842036	-0.850902062
C	-3.607147259	1.214351088	-1.024448074
C	-2.375631169	0.773464057	-0.487865037
C	0.183669015	0.880614063	-0.566764042
C	0.735520053	-0.264527018	-1.090559077
C	0.940522065	1.690681120	0.295938021
C	2.089636150	-0.590853043	-0.775326057
C	2.254332160	1.358531097	0.643119049
C	2.820380204	0.213160015	0.058832006
H	-1.444344104	-0.759299056	0.712433050
H	-3.501715254	-2.064002148	1.009193074
H	-5.615637401	-1.296207093	-0.001730002

H	-5.666343409	0.809073056	-1.289450092
H	-3.643936265	2.125836155	-1.585730115
C	-1.161100082	1.483672107	-0.760630054
O	-1.277463090	2.511836181	-1.635604119
H	2.507892180	-1.485787107	-1.194535088
H	2.823368204	1.948036140	1.334578095
O	4.101608295	-0.016888999	0.416629032
C	4.741155339	-1.181164086	-0.019295004
H	5.732596411	-1.156883084	0.406567029
H	4.820733347	-1.210210085	-1.100972079
H	4.225577305	-2.070395149	0.327959024
H	0.164512010	-0.921835065	-1.717998122
O	0.288168022	2.751130196	0.701835048
H	-0.485222035	3.029184217	-1.634029118
C	3.067683222	5.352814387	1.372228099
O	1.739038125	5.627416405	1.040245074
H	1.216120085	4.843053350	1.143235084
H	3.166642225	4.977625358	2.388343171
H	3.618180261	6.280996452	1.299226091
H	3.520353252	4.633827334	0.692455048
C	-4.325777313	6.012000432	-0.719186050
O	-4.156506302	4.641234334	-0.498944035
H	-3.236468232	4.419956317	-0.541970040
H	-5.383221388	6.221117448	-0.633618047
H	-3.995207287	6.310935454	-1.711337125
H	-3.799327275	6.612594474	0.017817001

Coord_11

C	-2.350761167	-0.374443027	0.289125023
C	-3.496397250	-1.144731084	0.436556032
C	-4.687357338	-0.750818054	-0.161471013
C	-4.730106340	0.434980031	-0.894892064
C	-3.607973257	1.208562085	-1.043926073
C	-2.377133170	0.810117059	-0.475050037
C	0.166869013	0.936008067	-0.530375036
C	0.694351048	-0.238868017	-1.028037076
C	0.966850068	1.773336129	0.278464022
C	2.040730145	-0.576448044	-0.742331051
C	2.289743167	1.423758104	0.596424041
C	2.815975201	0.249324020	0.046464001
H	-1.435407105	-0.690054049	0.753325053
H	-3.458607248	-2.054783150	1.005554071
H	-5.568687399	-1.355279096	-0.056286002
H	-5.649518409	0.742795055	-1.356790098
H	-3.659601266	2.114095151	-1.609303115
C	-1.162310083	1.548774112	-0.699807050
O	-1.279897093	2.657288189	-1.475996106

H	2.434374173	-1.490805110	-1.142669082
H	2.889311209	2.033293146	1.243366088
O	4.101909296	0.002066998	0.372538026
C	4.706362337	-1.189410086	-0.040804000
H	5.709287413	-1.170320085	0.357465026
H	4.756121345	-1.256405090	-1.122508079
H	4.184275301	-2.056086149	0.350657023
H	0.097197007	-0.904815063	-1.620619115
O	0.370394028	2.861562207	0.670085048
H	-0.493154037	3.185698232	-1.468380107
C	3.219514229	5.246622378	1.413747102
O	1.935205137	5.648731406	1.042550074
H	1.341533098	4.909859353	1.088045078
H	3.240689231	4.813144347	2.411118171
H	3.847722275	6.127163441	1.414182102
H	3.642432264	4.527167326	0.715414054
C	-4.473834324	5.955014430	-0.786882055
O	-4.290354310	4.592067333	-0.537092037
H	-3.365304244	4.383213318	-0.516361036
H	-5.538780396	6.142104443	-0.774072055
H	-4.084782295	6.249104448	-1.759078126
H	-4.010025287	6.576366471	-0.025349003

Coord_12

C	-2.348688168	-0.346580025	0.309182021
C	-3.477889249	-1.144456082	0.429283031
C	-4.661482333	-0.782934054	-0.199496013
C	-4.714047340	0.397824031	-0.938713068
C	-3.605172258	1.198893085	-1.060450077
C	-2.381017172	0.836452062	-0.456595033
C	0.148656012	0.984729072	-0.489160035
C	0.652621045	-0.217444017	-0.962436068
C	0.992206072	1.847551132	0.260277021
C	1.991990142	-0.564421041	-0.711230050
C	2.324729165	1.481547106	0.543573040
C	2.812299202	0.281862018	0.027078000
H	-1.439121104	-0.636113044	0.801157056
H	-3.432619247	-2.050586145	1.004179072
H	-5.530104398	-1.408431104	-0.112766010
H	-5.627939407	0.682539049	-1.425729104
H	-3.663930264	2.099170152	-1.629870118
C	-1.167377082	1.601588113	-0.631786046
O	-1.291656094	2.778845199	-1.302750094
H	2.361638172	-1.496066105	-1.093808077
H	2.955006215	2.109439154	1.142040080
O	4.103235293	0.018617001	0.316677023
C	4.673699337	-1.197095089	-0.075358005

H	5.688710408	-1.182452088	0.291131023
H	4.688806337	-1.300615092	-1.155149082
H	4.150300296	-2.041043148	0.361172024
H	0.029152004	-0.891305062	-1.517301110
O	0.450429033	2.959518213	0.636755047
H	-0.510401035	3.317861239	-1.286004095
C	3.333934241	5.173673373	1.457174107
O	2.095721149	5.669354406	1.047178073
H	1.456761105	4.967287356	1.026680075
H	3.278552238	4.684410340	2.427076173
H	4.009223287	6.014583431	1.540531113
H	3.753121269	4.470863321	0.739757054
C	-4.573860328	5.900473427	-0.850964060
O	-4.393642316	4.542621328	-0.576073043
H	-3.470087251	4.338278311	-0.492901037
H	-5.639099406	6.076819438	-0.909964064
H	-4.124672295	6.189784445	-1.798368129
H	-4.167128302	6.533912469	-0.067026003

Coord_13

C	-2.356243168	-0.331439025	0.332411024
C	-3.472343250	-1.150641084	0.421733032
C	-4.643503335	-0.814218061	-0.240418020
C	-4.697582339	0.362461026	-0.984650072
C	-3.598713258	1.185045088	-1.075553076
C	-2.387312170	0.850670060	-0.434037032
C	0.129623010	1.025310072	-0.443494033
C	0.611873042	-0.201784016	-0.893972063
C	1.015508075	1.911892138	0.241814016
C	1.944418139	-0.556312040	-0.681002049
C	2.357634169	1.530512110	0.486077037
C	2.808825201	0.309292021	0.002422002
H	-1.456855103	-0.600405041	0.854097059
H	-3.426408246	-2.053566148	1.001808072
H	-5.502170396	-1.455901102	-0.174847011
H	-5.602071403	0.629361043	-1.498597107
H	-3.656935266	2.081508152	-1.648245121
C	-1.176011085	1.639939117	-0.557844040
O	-1.312573095	2.874137204	-1.117637082
H	2.291395163	-1.503146111	-1.046752075
H	3.017468217	2.175118157	1.032772075
O	4.104505297	0.031360002	0.251911019
C	4.642948334	-1.205681085	-0.119750007
H	5.669968411	-1.194701086	0.211646018
H	4.619917333	-1.344054099	-1.195416083
H	4.123390294	-2.027057146	0.361873025
H	-0.037045000	-0.882881063	-1.408885101

O	0.526190038	3.043665216	0.601844043
H	-0.536376039	3.422575246	-1.088675079
C	3.416743247	5.139603370	1.498483107
O	2.218170161	5.693065410	1.048800076
H	1.559098111	5.014524363	0.960413071
H	3.293028237	4.599803333	2.434713174
H	4.108681294	5.953984428	1.666404118
H	3.857705278	4.464639324	0.767364056
C	-4.628040331	5.850607420	-0.906297067
O	-4.467438322	4.494506326	-0.613525044
H	-3.551480257	4.286488310	-0.469961034
H	-5.686933410	6.027790436	-1.035525077
H	-4.117712296	6.135080440	-1.823757132
H	-4.272486307	6.487802467	-0.100743008

Coord_14

C	-2.374453173	-0.330553024	0.356699026
C	-3.481392249	-1.164290084	0.411042032
C	-4.634731333	-0.844665062	-0.287242020
C	-4.681066336	0.329441021	-1.034966075
C	-3.588374257	1.167077086	-1.090816077
C	-2.395897171	0.851393059	-0.409050029
C	0.110495009	1.057095077	-0.393938028
C	0.573616041	-0.192788014	-0.822834061
C	1.036006073	1.965916139	0.223406014
C	1.899042137	-0.553028040	-0.650412048
C	2.387189173	1.570271112	0.425582029
C	2.805213201	0.330950023	-0.025467004
H	-1.489882108	-0.585222041	0.910136068
H	-3.442340249	-2.065088147	0.995125072
H	-5.486716393	-1.497269105	-0.246139018
H	-5.572051400	0.584728043	-1.577628115
H	-3.638477262	2.061737148	-1.665307118
C	-1.187879086	1.662187121	-0.479645036
O	-1.342804097	2.940938212	-0.922893065
H	2.225266158	-1.513113111	-0.999937071
H	3.074273220	2.230119163	0.917929065
O	4.104902296	0.039729003	0.181595015
C	4.614006334	-1.215937085	-0.170088014
H	5.652344406	-1.207741087	0.123914007
H	4.550802329	-1.387553098	-1.239263091
H	4.103104295	-2.015085146	0.355943028
H	-0.098984007	-0.880616063	-1.296194091
O	0.596041043	3.113818223	0.565182040
H	-0.570850042	3.496968254	-0.878933062
C	3.472851249	5.147005369	1.533460109
O	2.302502165	5.722798414	1.041349075

H	1.646443119	5.051859364	0.890137062
H	3.295350235	4.563959326	2.434479177
H	4.153563298	5.951016427	1.779401130
H	3.956418282	4.506004326	0.798573057
C	-4.638816333	5.806774419	-0.947867067
O	-4.512871327	4.449023319	-0.647113046
H	-3.610326260	4.228922303	-0.445976033
H	-5.684997410	5.996583430	-1.145002081
H	-4.067024292	6.086127438	-1.830009134
H	-4.328639310	6.439460463	-0.120229007

Coord_15

C	-2.374453173	-0.330553024	0.356699026
C	-3.481392249	-1.164290084	0.411042032
C	-4.634731333	-0.844665062	-0.287242020
C	-4.681066336	0.329441021	-1.034966075
C	-3.588374257	1.167077086	-1.090816077
C	-2.395897171	0.851393059	-0.409050029
C	0.110495009	1.057095077	-0.393938028
C	0.573616041	-0.192788014	-0.822834061
C	1.036006073	1.965916139	0.223406014
C	1.899042137	-0.553028040	-0.650412048
C	2.387189173	1.570271112	0.425582029
C	2.805213201	0.330950023	-0.025467004
H	-1.489882108	-0.585222041	0.910136068
H	-3.442340249	-2.065088147	0.995125072
H	-5.486716393	-1.497269105	-0.246139018
H	-5.572051400	0.584728043	-1.577628115
H	-3.638477262	2.061737148	-1.665307118
C	-1.187879086	1.662187121	-0.479645036
O	-1.342804097	2.940938212	-0.922893065
H	2.225266158	-1.513113111	-0.999937071
H	3.074273220	2.230119163	0.917929065
O	4.104902296	0.039729003	0.181595015
C	4.614006334	-1.215937085	-0.170088014
H	5.652344406	-1.207741087	0.123914007
H	4.550802329	-1.387553098	-1.239263091
H	4.103104295	-2.015085146	0.355943028
H	-0.098984007	-0.880616063	-1.296194091
O	0.596041043	3.113818223	0.565182040
H	-0.570850042	3.496968254	-0.878933062
C	3.472851249	5.147005369	1.533460109
O	2.302502165	5.722798414	1.041349075
H	1.646443119	5.051859364	0.890137062
H	3.295350235	4.563959326	2.434479177
H	4.153563298	5.951016427	1.779401130
H	3.956418282	4.506004326	0.798573057

C	-4.638816333	5.806774419	-0.947867067
O	-4.512871327	4.449023319	-0.647113046
H	-3.610326260	4.228922303	-0.445976033
H	-5.684997410	5.996583430	-1.145002081
H	-4.067024292	6.086127438	-1.830009134
H	-4.328639310	6.439460463	-0.120229007

Coord_16

C	-2.444574175	-0.374727026	0.398004031
C	-3.546190257	-1.215012088	0.366989026
C	-4.646321336	-0.900546063	-0.411021029
C	-4.646960333	0.274610019	-1.157141085
C	-3.554014254	1.120866079	-1.127752083
C	-2.418543174	0.809406056	-0.359439027
C	0.075247005	1.096959079	-0.286341022
C	0.509544038	-0.194163012	-0.672586051
C	1.067990075	2.046448148	0.187164013
C	1.818295129	-0.561232039	-0.581354041
C	2.433903173	1.624828117	0.302820024
C	2.797169199	0.357638025	-0.080828004
H	-1.604692113	-0.622233047	1.020409076
H	-3.545651253	-2.115791154	0.952811069
H	-5.495816395	-1.557513114	-0.431044032
H	-5.497873397	0.528447037	-1.761362129
H	-3.565965257	2.019721146	-1.698005123
C	-1.219909089	1.655394120	-0.319369022
O	-1.433158101	2.981726215	-0.517424037
H	2.110023154	-1.543333112	-0.897758067
H	3.165515226	2.311392168	0.681619048
O	4.101238294	0.043564004	0.040965003
C	4.561120328	-1.242866090	-0.268335020
H	5.618156407	-1.237718089	-0.051146002
H	4.417516317	-1.477977107	-1.317321096
H	4.078697296	-1.997868142	0.342582027
H	-0.202771017	-0.894618066	-1.060427079
O	0.715236049	3.217372231	0.484285037
H	-0.665785049	3.545320253	-0.438482031
C	3.517415255	5.282713378	1.563915111
O	2.369135169	5.805677419	0.973308067
H	1.773414130	5.102904367	0.737817053
H	3.286889236	4.644701334	2.414356175
H	4.112147294	6.114792441	1.916665137
H	4.119132296	4.711243341	0.859206059
C	-4.541555327	5.738456414	-0.967668070
O	-4.523600327	4.369800315	-0.691194050
H	-3.664595265	4.099703294	-0.387571026
H	-5.543209398	5.989307433	-1.288952094

H	-3.849139279	6.005605431	-1.762988126
H	-4.306603311	6.335955457	-0.090403006

Coord_17

C	-2.495284178	-0.419885028	0.407905027
C	-3.600171258	-1.251477089	0.325058021
C	-4.664430337	-0.924052064	-0.495010036
C	-4.627406334	0.255494020	-1.233000088
C	-3.528575254	1.094580078	-1.152199082
C	-2.431507175	0.766757053	-0.339519022
C	0.060539004	1.110219081	-0.230493015
C	0.484857035	-0.201015016	-0.592958041
C	1.080441076	2.077725148	0.168907012
C	1.783429127	-0.570664042	-0.538161038
C	2.451248175	1.642842120	0.244599017
C	2.792591202	0.364563029	-0.101874008
H	-1.685709124	-0.675512047	1.066323077
H	-3.631295263	-2.154809155	0.906302067
H	-5.517720396	-1.573895114	-0.552832038
H	-5.451623390	0.520609039	-1.868594136
H	-3.511561253	2.000319143	-1.713993124
C	-1.239656090	1.627324119	-0.243172017
O	-1.495027108	2.953609213	-0.315872023
H	2.061193148	-1.562523111	-0.835643061
H	3.199758228	2.340639170	0.565601043
O	4.096513297	0.039674001	-0.018775002
C	4.536079327	-1.260094090	-0.302836021
H	5.599923404	-1.256031088	-0.122066009
H	4.355321311	-1.527028107	-1.338301095
H	4.070579294	-1.991772142	0.348122026
H	-0.243219018	-0.907252067	-0.937953069
O	0.765608056	3.256711236	0.437665029
H	-0.727312054	3.516584251	-0.220061015
C	3.510562251	5.402551387	1.546460110
O	2.364378168	5.858430422	0.899404067
H	1.815589128	5.121982366	0.653719046
H	3.275790235	4.760585341	2.392813174
H	4.044577291	6.267838449	1.916199138
H	4.172891302	4.857402351	0.875890066
C	-4.441838320	5.712161411	-0.932643066
O	-4.492957324	4.336986314	-0.693765047
H	-3.663608265	4.028958291	-0.348309027
H	-5.411584389	6.011183430	-1.306377096
H	-3.692338266	5.971963432	-1.677095118
H	-4.238189303	6.277270452	-0.026466001

Coord_18

C	-2.553525183	-0.479596034	0.404084028
C	-3.664155265	-1.294601093	0.262374018
C	-4.686508337	-0.943443066	-0.599218044
C	-4.603805331	0.243673015	-1.321358094
C	-3.496672253	1.067974078	-1.182555087
C	-2.444551177	0.710792050	-0.327077023
C	0.048124003	1.126350081	-0.175606015
C	0.464168036	-0.206288013	-0.509741034
C	1.091955078	2.108983151	0.149418012
C	1.750961123	-0.579942043	-0.485027033
C	2.465449175	1.658402117	0.191367014
C	2.787089198	0.369903025	-0.113150008
H	-1.779514125	-0.751480055	1.097968077
H	-3.734036269	-2.202567158	0.833130062
H	-5.545802399	-1.580012112	-0.700356051
H	-5.397235388	0.528348039	-1.986984141
H	-3.445729248	1.984562144	-1.729370125
C	-1.262052088	1.585571114	-0.175075012
O	-1.569954114	2.893248208	-0.123721011
H	2.016017144	-1.581589113	-0.759935053
H	3.228037232	2.365088170	0.454802032
O	4.089018295	0.032729004	-0.062480005
C	4.509760326	-1.280046094	-0.315760022
H	5.578600402	-1.278161090	-0.167524012
H	4.295935310	-1.580213115	-1.335632094
H	4.059960294	-1.985717142	0.373663025
H	-0.277540021	-0.917267064	-0.812558058
O	0.812410058	3.294565237	0.383874030
H	-0.799879056	3.453016247	-0.014892000
C	3.489762251	5.546253400	1.496942105
O	2.348639171	5.917068426	0.789285055
H	1.848569132	5.142244372	0.560707042
H	3.254367235	4.923656353	2.357539171
H	3.963585284	6.451158466	1.853815136
H	4.205950301	5.012816359	0.873756063
C	-4.317600313	5.687636411	-0.856590061
O	-4.443810320	4.308001308	-0.675934050
H	-3.648615260	3.953751282	-0.298007020
H	-5.249427377	6.045856436	-1.272419094
H	-3.514940251	5.939793429	-1.546323111
H	-4.142148299	6.208434445	0.081572006

Coord_19

C	-2.611519188	-0.702909050	0.416026030
C	-3.722309267	-1.494049109	0.177638013
C	-4.717291340	-1.066234074	-0.680956047
C	-4.610116330	0.174598012	-1.303421096

C	-3.500459252	0.977342070	-1.068714079
C	-2.479381179	0.536197039	-0.217655016
C	0.011367002	1.067394078	-0.025149001
C	0.430194031	-0.263202021	-0.412811029
C	1.069974077	2.056642150	0.269899019
C	1.707696121	-0.627418047	-0.452347031
C	2.449073177	1.602946114	0.237246015
C	2.762397200	0.326607023	-0.102378007
H	-1.861971133	-1.034032072	1.111184078
H	-3.815631273	-2.442894175	0.673873047
H	-5.578295400	-1.684541124	-0.855018061
H	-5.384957386	0.519255038	-1.962581143
H	-3.432964249	1.941186141	-1.534327113
C	-1.317771092	1.427928105	0.023350999
O	-1.702131123	2.677761194	0.278511019
H	1.967895141	-1.619117115	-0.764833054
H	3.219111229	2.310687166	0.475157036
O	4.064676295	-0.010627001	-0.116938007
C	4.478374320	-1.315829096	-0.418769030
H	5.552343400	-1.312456094	-0.314319025
H	4.224321303	-1.592607112	-1.435949104
H	4.060354293	-2.039750145	0.271593021
H	-0.319766021	-0.969083069	-0.706132052
O	0.813908058	3.230410232	0.539201041
H	-0.932742065	3.234980234	0.413852032
C	3.407998244	5.554712399	1.730660122
O	2.266502163	5.865824420	0.994396072
H	1.813629130	5.062804363	0.770384055
H	3.183386230	4.924698356	2.588815188
H	3.828472278	6.483168467	2.094007149
H	4.164198300	5.054511362	1.127197082
C	-4.269606307	5.545711401	-0.280331018
O	-4.454673318	4.160483302	-0.263649017
H	-3.685316264	3.738294267	0.095327006
H	-5.171266374	5.988058432	-0.681470048
H	-3.433295245	5.840904420	-0.910528066
H	-4.108574294	5.948627430	0.716704050