

Quantum mechanics/molecular mechanics studies on excited state decay pathways of 5-azacytosine in aqueous solution

Xue-Ping Chang,^{a*} Lingyun Zheng,^a Li Yu,^a Teng-Shuo Zhang^b and Bin-Bin Xie^c

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

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

^c Hangzhou Institute of Advanced Studies, Zhejiang Normal University, Hangzhou 311231, P. R. China.

E-mail: xuepingchang@xynu.edu.cn

Contents

1. Active Orbitals
2. Bond-Lengths of Minima and Intersection Structures
3. QM(CASSCF)/MM Optimized Intersection Structures
4. QM(CASPT2)/MM Computed LIICs
5. Tables
6. QM(CASPT2)/MM Computed Relaxation Pathways II' and III'
7. Cartesian Coordinates of All Computed Structures

1. Active Orbitals

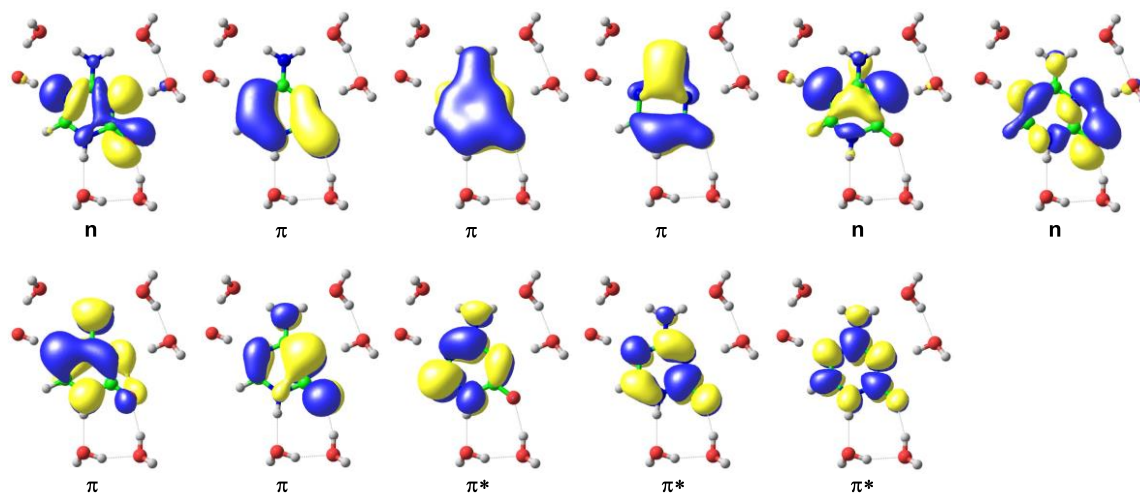


Figure S1. Molecular orbitals (MOs) included in the active space used for QM/MM calculations.

2. Bond-Lengths of Minima and Intersection Structures

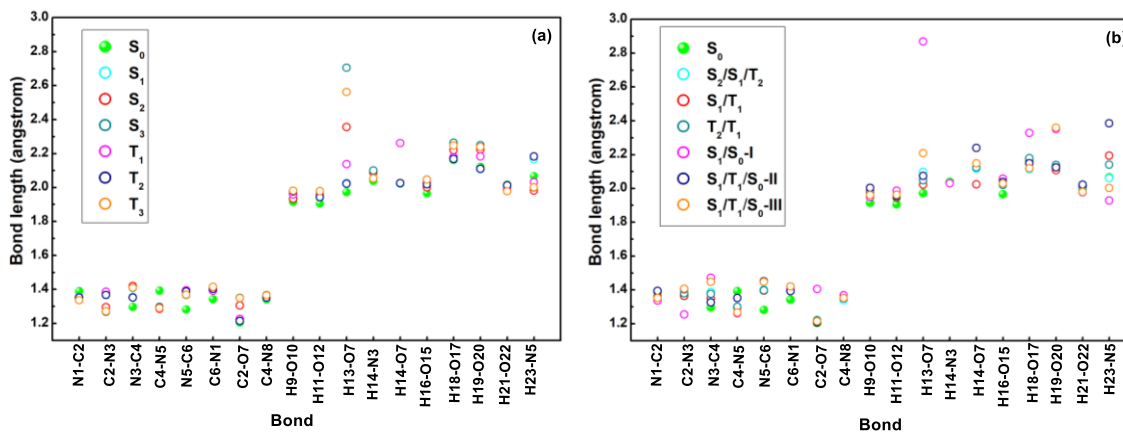


Figure S2. QM(CASSCF)/MM computed bond-lengths (in Å) of (a) minima and (b) conical intersections and crossing points in and between S₀, S₁, S₂, S₃, T₁, T₂, and T₃ states.

3. QM(CASSCF)/MM Optimized Intersection Structures

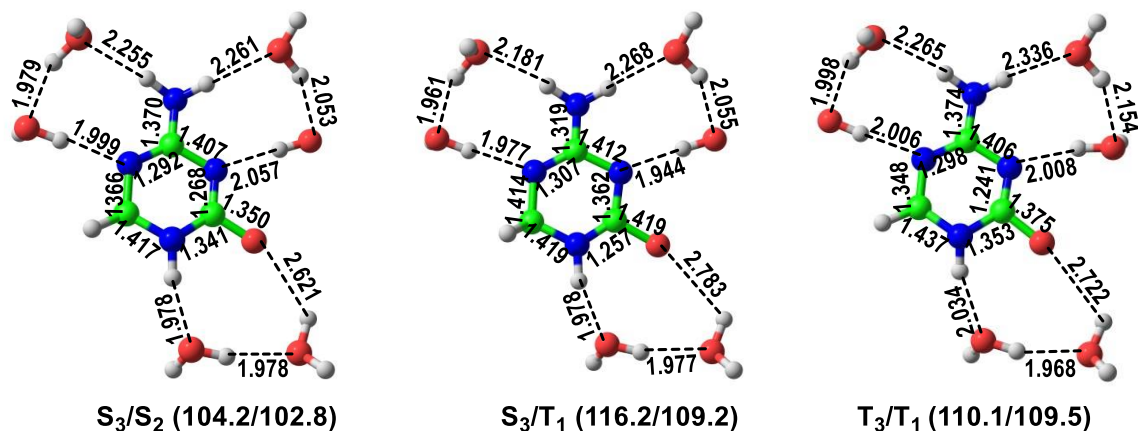


Figure S3. QM(CASSCF)/MM optimized minimum-energy conical intersections and crossing points between S_3 , S_2 , and T_1 states together with relative energies in kcal/mol at the QM(CASPT2)/MM level.

4. QM(CASPT2)/MM Computed LIICs

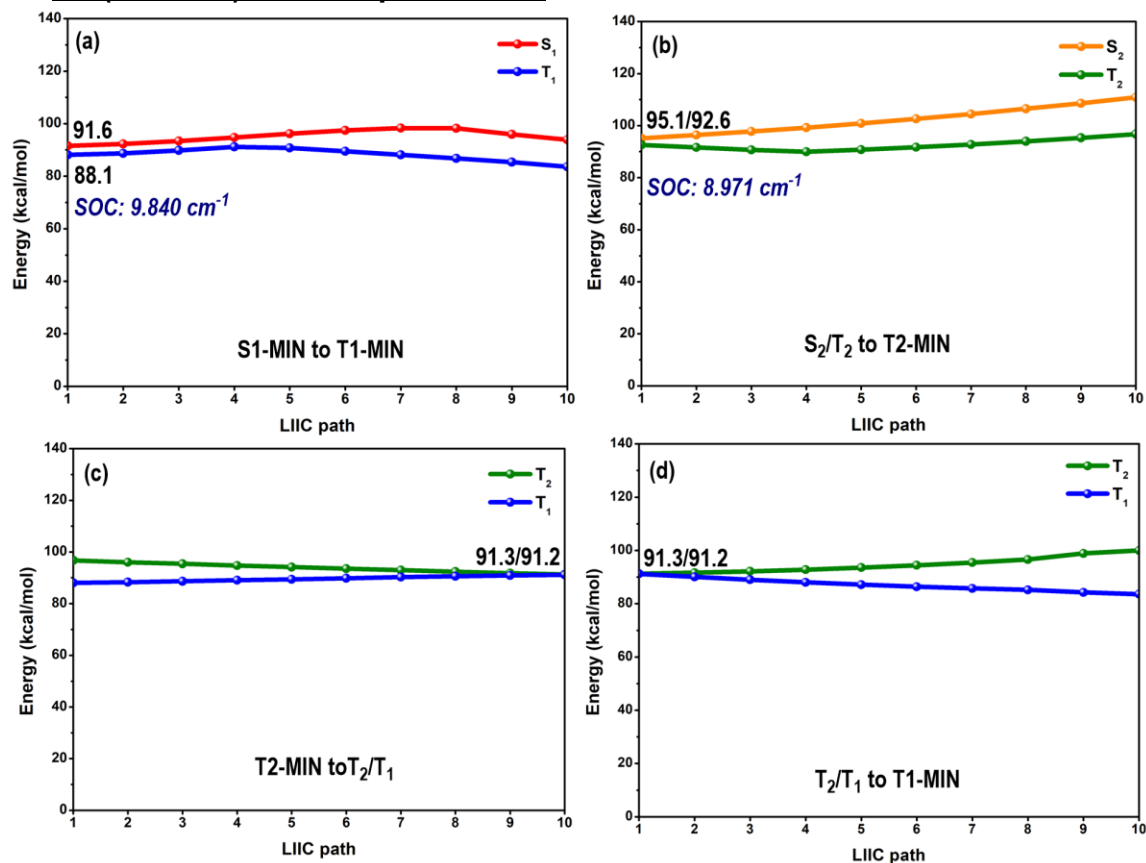


Figure S4. QM(CASPT2)/MM computed LIICs (in kcal/mol) connecting (a) S_1 -MIN and T_1 -MIN, (b) S_2/T_2 and T2-MIN, (c) T2-MIN and T_2/T_1 , and (d) T_2/T_1 and T1-MIN.

5. Tables

Table S1: Optimized geometrical parameters of S_0 minimum of 5-AC

	This work	DFT ^a	CASSCF ^b	CASSCF ^c
N1-C2	1.389	1.417	1.403	1.403
C2-N3	1.366	1.362	1.386	1.349
N3-C4	1.298	1.333	1.281	1.288
C4-N5	1.393	1.385	1.397	1.346
N5-C6	1.282	1.304	1.279	1.288
C6-N1	1.343	1.346	1.351	1.340
C2=O7	1.204	1.230	1.193	1.236
C4-N8	1.340	1.340	1.369	1.342

^a *J. Phys. Chem. A* 2009, 113, 12088-12093. ^b *J. Chem. Theory Comput.* 2014, 10, 3915-3924.

^c *Phys. Chem. Chem. Phys.*, 2017, 19, 5888-5894.

Table S2: The vertical excitation energies (in eV) of $^1n_{\text{N}\pi^*}$, $^1\pi\pi^*$, $^1n_{\text{O}\pi^*}$, and $^3\pi\pi^*$ states at Franck-Condon point of 5-AC

	$^1n_{\text{N}\pi^*}$	$^1\pi\pi^*$	$^1n_{\text{O}\pi^*}$	$T_1(^3\pi\pi^*)$
SS-CASPT2(14,10)/ANO-L ^a	4.46	4.74	5.58	4.33
MS-CASPT2(14,10)/ANO-L ^b	4.61	5.06	-	-
MRCIS(6,5)/def2-SVP ^b	5.07	5.31	-	4.62
TDDFT ^c		4.66, 5.00	-	4.03
This work	4.86	4.88, 6.18	5.10	4.51
Exp. ^c		4.77, 5.51		
Exp. ^d		5.17, 6.17		

^a *J. Chem. Theory Comput.* 2014, 10, 3915-3924. ^b *Phys. Chem. Chem. Phys.*, 2017, 19, 5888-5894.

^c *J. Phys. Chem. A* 2009, 113, 12088-12093. ^d *J. Phys. Chem. A* 2017, 121, 2780-2789.

Table S3: The computed adiabatic excitation energies (in eV) of the minima and intersection structures of 5-AC

	SS-CASPT2(14,10)/ANO-L ^a	MS-CASPT2(14,10)/ANO-L ^b	MRCIS(6,5)/def2-SVP ^b	This work	
S_0 min	0.00	0.00	0.00	S0-MIN	0.00
$^1n_{\text{N}\pi^*}$ min	3.59	-	4.10	S1-MIN	3.97
$^1\pi\pi^*$ min	3.69	-	4.28	S2-MIN	4.12
$^3\pi\pi^*$ min	3.27	-	3.54	T1-MIN	3.63
$^1\pi\pi^*/^1n_{\text{N}\pi^*}$ CoIn	4.04/ 3.97	-	4.41/4.41	S ₂ /S ₁	4.12/4.12
S ₁ /S ₀ CoIn (a)	3.87/ 3.75	4.83/4.82	5.31/5.31	S ₁ /S ₀ -I	4.30/3.95
S ₁ /S ₀ CoIn (b)	3.47/ 3.47/3.89(T1)	3.77/3.76	4.06/4.06	S ₁ /T ₁ /S ₀ -II	4.21/4.08
S ₁ /S ₀ CoIn (γ)	-	3.85/3.84	3.99/3.99	S ₁ /T ₁ /S ₀ -III	3.75/3.75
$^1\pi\pi^*/^3\pi\pi^*$ STC	3.87/ 3.89/ 3.77(T1)	-	-	-	-
$^1n_{\text{N}\pi^*}/^3\pi\pi^*$ STC	-	-	4.12/4.12	S ₁ /T ₁	3.95/3.89
$^3\pi\pi^*/^3\pi\pi^*$	-	-	-	T ₂ /T ₁	3.96/3.95

^a *J. Chem. Theory Comput.* 2014, 10, 3915-3924. ^b *Phys. Chem. Chem. Phys.*, 2017, 19, 5888-5894.

6. QM(CASPT2)/MM Computed Relaxation Pathways II' and III'

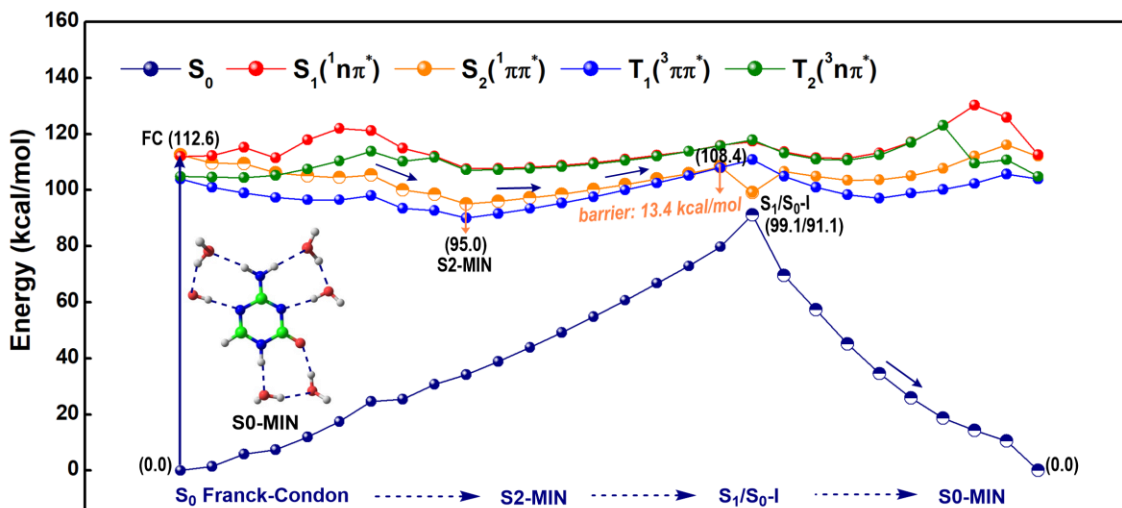


Figure S5. Relaxation pathway II' of 5-AC in aqueous solution computed at the QM(CASPT2)/MM level. Relative energies of minima and intersection structures are in kcal/mol.

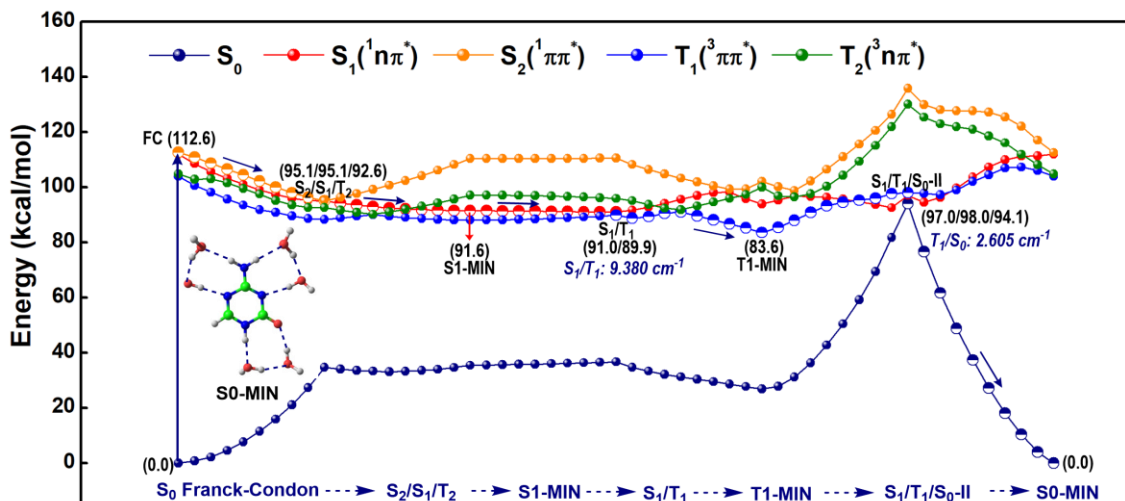


Figure S6. Relaxation pathway III' of 5-AC in aqueous solution computed at the QM(CASPT2)/MM level. Spin-orbital couplings at S_1/T_1 and $S_1/T_1/S_0-II$ are given in cm^{-1} . Relative energies of minima and intersection structures are in kcal/mol.

7. Cartesian coordinates of All Computed Structures

In xyz format (unit: Ångstrom)

CASSCF/ANO-L-VDZP

S0-MIN

C	-0.357476028	-0.325875023	0.229680018
N	0.341885027	-0.973917071	1.110492078
C	1.653274120	-0.646333049	1.306678092
C	1.358668096	1.022653073	-0.350634025
N	0.124605007	0.729787053	-0.539943037
N	2.151526155	0.392262029	0.530966037
H	3.102758223	0.691790052	0.672735046
N	-1.649147119	-0.620508046	0.029419001
H	-1.963775141	-1.512845109	0.364878027
H	-2.065503149	-0.287993023	-0.820383060
H	1.807123128	1.824952131	-0.918745067
O	2.363013171	-1.219113085	2.093251151
O	-2.733839197	0.356619025	-2.728166195
H	-2.629401188	-0.143525009	-3.525973252
H	-2.360519169	1.219526087	-2.880668210
O	-1.191319087	2.765921198	-2.329191167
H	-1.566105111	3.489871251	-1.844840131
H	-0.810044059	2.169065158	-1.692877120
O	4.862872351	1.248671090	1.181207087
H	5.136525369	2.113660152	1.453307107
H	5.132414370	0.636409044	1.865785136
O	-2.145668152	-3.642177264	0.683196049
H	-2.886480206	-4.220391304	0.804450057
H	-1.559679111	-3.776041274	1.425256104
O	5.025804364	-0.758670055	3.159791227
H	4.140683299	-1.031827075	2.927287212
H	5.552154399	-1.544063112	3.226183233
O	-0.264665017	-3.327435241	2.832781203
H	-0.002365999	-2.522987184	2.391665171
H	0.533658036	-3.727547270	3.149010225

S1-MIN

C	-0.528514036	-0.198852015	0.053044002
N	0.272746019	-0.910152065	0.884654066
C	1.562816111	-0.642046047	1.248051090
C	1.456630102	0.873824062	-0.582809040
N	0.070876006	0.748146053	-0.594151045
N	2.110098154	0.394877027	0.566599039
H	3.079049219	0.607218045	0.725546052

N	-1.853804134	-0.459780034	0.017630000
H	-2.085728150	-1.385158100	0.332370023
H	-2.292495164	-0.199327015	-0.848195061
H	1.847113132	1.792133130	-0.988200073
O	2.132379151	-1.281374091	2.107923151
O	-2.789862203	0.433758029	-2.797952202
H	-2.500767179	-0.039636000	-3.565975258
H	-2.439824174	1.317267093	-2.865880208
O	-1.341935098	2.902234209	-2.304437165
H	-1.692337122	3.660765265	-1.855336134
H	-0.901531063	2.370124170	-1.651441118
O	4.913998355	1.132336081	1.249375092
H	5.124980367	2.000144144	1.565857113
H	5.128620371	0.515414037	1.946282139
O	-1.803395127	-3.468521251	0.881142065
H	-2.442738174	-4.155033300	1.014047074
H	-1.175779083	-3.528008256	1.597332115
O	4.875443353	-0.958641068	3.189077229
H	3.977989288	-1.155925083	2.933095212
H	5.358459386	-1.774142130	3.157625225
O	0.244686019	-3.374689245	3.029956218
H	0.891092063	-2.702802195	2.833502202
H	0.717654050	-4.099522294	3.415423246

S2-MIN

C	-0.373591026	-0.216509014	0.096070008
N	0.391908030	-1.007749071	0.993653070
C	1.592742116	-0.571826041	1.213374089
C	1.499077108	0.898384062	-0.590315044
N	0.118952008	0.714147050	-0.641966046
N	2.155088153	0.470830033	0.562369040
H	3.111154223	0.715774053	0.752050053
N	-1.697154121	-0.504147038	0.118751010
H	-1.929674139	-1.434006103	0.412078029
H	-2.207295161	-0.190024015	-0.686825052
H	1.899777138	1.775449129	-1.067684078
O	2.324976169	-1.146852085	2.127243153
O	-2.842168205	0.383047026	-2.740070196
H	-2.509548182	-0.156216013	-3.444381249
H	-2.414772172	1.231371090	-2.817512201
O	-1.196135087	2.720983196	-2.330915168
H	-1.509102106	3.451587251	-1.814755129
H	-0.772810058	2.110702152	-1.728699123
O	4.914020353	1.165513081	1.289280094
H	5.203465375	2.049216147	1.471849108
H	5.220375377	0.610337042	2.002503142
O	-2.284770166	-3.608108261	0.685903050

H	-2.832611205	-4.362884312	0.518890038
H	-1.676933121	-3.839280279	1.382490100
O	5.237757378	-0.776232056	3.396705247
H	4.363718317	-1.136281081	3.308363238
H	5.833102422	-1.512325108	3.468175248
O	-0.184234012	-3.475678252	2.664271191
H	0.055879006	-2.686603196	2.188077158
H	-0.394389030	-3.202874230	3.547525255

S3-MIN

C	-0.430106029	-0.183603016	0.152699011
N	0.365636026	-0.882344065	1.082527077
C	1.588114112	-0.544012040	1.079117080
C	1.305479093	1.194079085	-0.446458034
N	0.005357999	0.789886057	-0.575690040
N	2.181490155	0.355906028	0.280863021
H	3.103711223	0.676832047	0.515766035
N	-1.744239128	-0.560962042	0.139462008
H	-1.898169138	-1.526102111	0.364448028
H	-2.231410160	-0.275115018	-0.690814048
H	1.748263124	1.743828126	-1.258459091
O	2.405961175	-1.174706086	1.949572140
O	-2.841416207	0.306176024	-2.776364199
H	-2.471928178	-0.213952013	-3.476461249
H	-2.457176177	1.175122083	-2.847929204
O	-1.310047094	2.721723197	-2.375640171
H	-1.650796120	3.471384248	-1.906265137
H	-0.908209063	2.144568157	-1.729085126
O	4.852132349	1.092770080	1.316734095
H	5.134673370	1.972380140	1.528787109
H	5.159531371	0.517304036	2.012657143
O	-2.107691154	-3.756463272	0.691515049
H	-2.927051209	-4.220352304	0.800354056
H	-1.643838117	-3.802368276	1.522065108
O	5.377894389	-0.894416064	3.363987244
H	4.537594324	-1.258868092	3.612018262
H	5.962977431	-1.628073117	3.218403232
O	-0.320736024	-3.204300230	2.930281212
H	-0.128583007	-2.419829175	2.424460174
H	0.481005032	-3.707822268	2.965432213

T1-MIN

C	-0.423898028	-0.152036010	0.053306003
N	0.319811022	-0.996880072	0.905004064
C	1.620508115	-0.606153044	1.180635083
C	1.489371108	0.936257066	-0.624707046
N	0.107005006	0.759349053	-0.687253050

N	2.169131157	0.388648029	0.461328031
H	3.110036225	0.672011047	0.668896050
N	-1.759399125	-0.405889031	0.087894007
H	-1.987531141	-1.344138095	0.363768025
H	-2.262516162	-0.086644006	-0.720380054
H	1.870221133	1.872892134	-0.993036070
O	2.195130159	-1.198825086	2.086624153
O	-2.870002208	0.416966028	-2.755116198
H	-2.577399183	-0.113193009	-3.483789253
H	-2.472259178	1.276549089	-2.859336207
O	-1.273743090	2.788246202	-2.379464170
H	-1.571062111	3.520601251	-1.856362135
H	-0.814580060	2.190624157	-1.794270127
O	4.907009353	1.193007083	1.250597089
H	5.165241373	2.066870151	1.510222110
H	5.169779370	0.597335041	1.948988140
O	-1.908706136	-3.461944250	0.868896062
H	-2.353677172	-4.294625310	0.785986058
H	-1.276836094	-3.549353256	1.577374116
O	5.005178363	-0.855862061	3.243423235
H	4.115876295	-1.110795080	3.020890216
H	5.519218396	-1.651977117	3.290351235
O	0.129721008	-3.457999249	3.051432221
H	0.705336053	-2.771724198	2.735364196
H	-0.116294008	-3.217004231	3.935135281

T2-MIN

C	-0.523438036	-0.197572014	0.062985005
N	0.271008021	-0.896583066	0.906102065
C	1.572471114	-0.637488047	1.239901088
C	1.455305106	0.887513063	-0.590476041
N	0.075146006	0.738650052	-0.601153044
N	2.128303153	0.368422027	0.527469038
H	3.093328221	0.593078042	0.693032052
N	-1.848773135	-0.461649036	0.022822002
H	-2.079924150	-1.386961102	0.338974023
H	-2.286014166	-0.202093014	-0.843988059
H	1.830797132	1.825770133	-0.963882071
O	2.142177154	-1.268604091	2.107309152
O	-2.780555198	0.430916030	-2.795451199
H	-2.482203181	-0.043150002	-3.559686256
H	-2.438437174	1.317243095	-2.865619208
O	-1.346122097	2.912755211	-2.305690167
H	-1.696506123	3.669207262	-1.853003134
H	-0.897228064	2.382873172	-1.657166118
O	4.911818351	1.134911084	1.249448092
H	5.120531367	2.004170146	1.563281115

H	5.127314367	0.520483036	1.948387138
O	-1.798910128	-3.467212252	0.884225062
H	-2.420342175	-4.173117303	1.001618071
H	-1.166579083	-3.529341254	1.596155114
O	4.881255349	-0.954130070	3.190952231
H	3.984267288	-1.150213080	2.932180212
H	5.365362387	-1.768672125	3.152018227
O	0.255287017	-3.371531242	3.021043217
H	0.900819066	-2.697098193	2.828276201
H	0.722873051	-4.081597293	3.439601249

T3-MIN

C	-0.454636035	-0.157952011	0.144729009
N	0.332282026	-0.869313064	1.074972077
C	1.559470112	-0.539083040	1.072794078
C	1.294450092	1.204698085	-0.453532033
N	-0.009846999	0.810197060	-0.584016041
N	2.157783157	0.356674028	0.281121021
H	3.085842220	0.661008050	0.514390036
N	-1.770422130	-0.525993036	0.130751009
H	-1.931430140	-1.489739109	0.357689027
H	-2.257933164	-0.236853016	-0.698089050
H	1.745291127	1.736187124	-1.273517094
O	2.379610170	-1.164667086	1.941557142
O	-2.875984208	0.335169027	-2.772926198
H	-2.522050180	-0.186562016	-3.479499250
H	-2.486310179	1.201320088	-2.849537204
O	-1.331390098	2.739194196	-2.386323169
H	-1.659603122	3.494852254	-1.918021137
H	-0.921707068	2.165551156	-1.741673126
O	4.852755349	0.990360069	1.346851097
H	5.152544374	1.840758132	1.638082118
H	5.149166371	0.348221025	1.987382146
O	-2.093028150	-3.704464267	0.703671050
H	-2.681839193	-4.444099320	0.638767047
H	-1.577864113	-3.814927277	1.497156110
O	5.330934385	-1.182628087	3.229086231
H	4.479213320	-1.585174114	3.347699242
H	5.946946429	-1.888258135	3.076711219
O	-0.309437021	-3.125441226	2.947267214
H	-0.143688012	-2.361534168	2.402259173
H	-0.701224049	-2.804408201	3.748733268

S₂/S₁/T₂

C	-0.451273034	-0.206392013	0.003103000
N	0.335008024	-1.025556076	0.800971056
C	1.561200115	-0.634017047	1.249789088

C	1.504268109	0.801837060	-0.576528040
N	0.103719005	0.776500058	-0.629494047
N	2.086553148	0.474402033	0.654833049
H	3.051260222	0.693035047	0.829636058
N	-1.761930126	-0.481940035	-0.002097002
H	-2.016053144	-1.396358100	0.328027023
H	-2.290486164	-0.124101008	-0.777553057
H	1.994073142	1.580866114	-1.135219081
O	2.132567152	-1.260817089	2.127673152
O	-2.838203206	0.497246038	-2.731611197
H	-2.537536182	-0.004727003	-3.476592252
H	-2.441886177	1.360718096	-2.801908204
O	-1.257381088	2.873063207	-2.287704162
H	-1.536893109	3.643065260	-1.810262128
H	-0.797474057	2.310325167	-1.670300122
O	4.915076353	1.160494084	1.263647092
H	5.156067371	2.031405147	1.548772112
H	5.158310374	0.554636041	1.960138143
O	-1.928169138	-3.446720249	0.836115061
H	-2.584562185	-4.117765299	0.966918067
H	-1.286629091	-3.539599254	1.536491109
O	4.935176357	-0.916059064	3.232391234
H	4.031943290	-1.122353083	3.011176215
H	5.419615390	-1.731207127	3.208732232
O	0.132418007	-3.422491244	2.982061216
H	0.753433053	-2.739870199	2.750735197
H	0.630725045	-4.109244296	3.403984244

S₁/T₁

C	-0.533673038	-0.207645014	0.062313002
N	0.262369017	-0.902803063	0.904136065
C	1.554121109	-0.633366047	1.254824088
C	1.454543107	0.858796063	-0.585176040
N	0.063997003	0.754815052	-0.570179040
N	2.098345148	0.418020028	0.582824043
H	3.074295223	0.610300042	0.724124052
N	-1.857491134	-0.469087034	0.015601003
H	-2.093587152	-1.389462100	0.341863023
H	-2.289872165	-0.216321018	-0.855486060
H	1.854996132	1.752325125	-1.033960072
O	2.134961155	-1.274335091	2.105551151
O	-2.764036200	0.430891031	-2.804599202
H	-2.478059178	-0.035569003	-3.578125258
H	-2.418954175	1.316614094	-2.868257209
O	-1.347239095	2.921258211	-2.297742168
H	-1.714106124	3.688796266	-1.877729137
H	-0.913591066	2.413792173	-1.621395117

O	4.918200356	1.125437081	1.243343090
H	5.121926368	1.993323145	1.564308110
H	5.130001370	0.507962036	1.940628140
O	-1.808420131	-3.475823251	0.887045064
H	-2.432870177	-4.176843303	1.015764075
H	-1.174654084	-3.531735252	1.598187117
O	4.875291352	-0.963333071	3.186660228
H	3.977214287	-1.156588084	2.929736212
H	5.355607385	-1.780278130	3.151695228
O	0.250223018	-3.376738241	3.022790216
H	0.891209064	-2.700111196	2.824264201
H	0.725182052	-4.087664295	3.431151246

T_2/T_1

C	-0.481122033	-0.200337013	0.087795009
N	0.310631025	-0.959914067	0.918946064
C	1.616299119	-0.629660044	1.222086088
C	1.469722106	0.906628067	-0.578271044
N	0.078042008	0.772841057	-0.567760038
N	2.142450157	0.423339032	0.547989040
H	3.110320224	0.647317049	0.697115052
N	-1.816529132	-0.470197031	0.069111004
H	-2.057527146	-1.408435099	0.350851025
H	-2.285070167	-0.180279015	-0.771549055
H	1.856139134	1.815258133	-1.007523070
O	2.208162160	-1.270138091	2.077192150
O	-2.810984202	0.463666032	-2.743277195
H	-2.526741183	-0.006348000	-3.515281252
H	-2.452660178	1.342722096	-2.803558199
O	-1.348297095	2.915883209	-2.241722163
H	-1.701981123	3.660939264	-1.773874128
H	-0.888927061	2.376021173	-1.606024116
O	4.943400354	1.141648082	1.244711087
H	5.169183373	2.005572143	1.561671114
H	5.179072373	0.516277035	1.926856138
O	-1.872232134	-3.532496256	0.805691057
H	-2.402457175	-4.318351311	0.802108056
H	-1.235569090	-3.610496258	1.502823106
O	4.969427360	-0.975730069	3.162556226
H	4.072799293	-1.187898083	2.919762211
H	5.462683396	-1.785603130	3.139610227
O	0.195038012	-3.421536249	2.917383210
H	0.786087057	-2.721068198	2.698070197
H	0.383311027	-3.865308280	3.735569269

S_1/S_0-I

C	-0.412763027	-0.198008014	0.034189004
N	0.405097027	-1.056480078	0.906308063
C	1.516807107	-0.526772038	1.149285083
C	1.516957108	0.748820056	-0.716934052
N	0.067351003	0.727846052	-0.674833049
N	2.103976150	0.508137035	0.540272037
H	3.030796218	0.799438056	0.788131057
N	-1.749006126	-0.432124030	0.219997017
H	-1.954863140	-1.392721101	0.418584030
H	-2.303200166	-0.089682007	-0.543891038
H	1.940422142	1.581051114	-1.255276090
O	2.351911170	-1.075651080	2.137841155
O	-2.870726207	0.425988029	-2.766074199
H	-2.402418175	-0.142367011	-3.361889241
H	-2.421135174	1.266280093	-2.786699200
O	-1.206202086	2.744934198	-2.293296164
H	-1.517070108	3.476532248	-1.777719130
H	-0.783142058	2.131773154	-1.688415119
O	4.861567352	1.111179082	1.378857102
H	5.230761375	1.974148142	1.508285110
H	5.176342374	0.552358038	2.083569149
O	-2.275856164	-3.683598263	0.681468048
H	-2.807469200	-4.447300318	0.502444035
H	-1.641552119	-3.922996283	1.349164099
O	5.450944392	-0.887440063	3.423129247
H	4.684658339	-1.309065095	3.791900272
H	6.107292438	-1.564321112	3.317193237
O	-0.178674015	-3.374133244	2.689807195
H	-0.030319004	-2.629336189	2.113399151
H	-0.616389046	-3.033691220	3.458318248

S₁/T₁/S₀-II

C	-0.542679037	-0.313289024	0.155888013
N	0.271979019	-1.056551078	0.892797062
C	1.549357112	-0.594863042	1.246452091
C	1.348649098	0.646652048	-0.561765042
N	-0.026274000	0.894693067	-0.165181011
N	2.014081144	0.581812044	0.660302048
H	2.994884218	0.779150056	0.760245056
N	-1.852298133	-0.619415046	0.041062001
H	-2.072390147	-1.562821112	0.309467020
H	-2.284787163	-0.304507020	-0.807365057
H	1.746071124	0.978772071	-1.500164107
O	2.190152157	-1.222662086	2.055813146
O	-2.498641178	0.572666041	-2.731083195
H	-2.336800169	0.206473014	-3.590335261
H	-2.159778155	1.463796104	-2.729688199

O	-1.232392090	3.126873227	-2.046259147
H	-1.667943119	3.960723288	-1.927594139
H	-0.925171067	2.850878203	-1.191430088
O	4.906577354	1.166705085	1.221135087
H	5.139989368	2.029385145	1.536289112
H	5.143999373	0.543479037	1.904202139
O	-1.927764137	-3.653831265	0.783632055
H	-2.535338181	-4.361271316	0.955511069
H	-1.281447091	-3.668203264	1.486016109
O	4.965363358	-0.932913068	3.176402228
H	4.063382293	-1.131146083	2.943686214
H	5.446320394	-1.749595126	3.140434225
O	0.117196007	-3.450725248	2.952999215
H	0.611185043	-2.708221192	2.620999187
H	0.741587055	-4.028244288	3.372324241

S₁/T₁/S₀-III

C	-0.279066020	-0.221724018	-0.067443005
N	0.576741039	-1.195788084	0.576110043
C	1.644928116	-0.617284044	1.285418095
C	1.700646120	0.491885033	-0.685399051
N	0.267707018	0.679219050	-0.769785053
N	2.169191155	0.458764035	0.655589047
H	3.109632225	0.735103051	0.871959062
N	-1.589551114	-0.390287028	0.223329018
H	-1.856962132	-1.348902098	0.364873026
H	-2.202189156	0.101146008	-0.402471027
H	2.300010164	1.050128078	-1.382207101
O	2.008146145	-1.141668085	2.318607167
O	-2.846417207	0.488158038	-2.638677189
H	-2.552359183	-0.057574003	-3.355138241
H	-2.399043172	1.324826094	-2.729082196
O	-1.127765080	2.778486199	-2.297183166
H	-1.301762094	3.556863255	-1.785377129
H	-0.611774044	2.187477155	-1.750850129
O	4.959872355	1.192614085	1.331232097
H	5.193482372	2.082156151	1.559083115
H	5.180235372	0.639821047	2.077220149
O	-1.929670138	-3.406028244	0.871079061
H	-2.349978170	-4.240188307	0.711322053
H	-1.295928095	-3.534091255	1.571384115
O	4.888650352	-0.722688050	3.459663247
H	3.972543287	-0.927002068	3.306458237
H	5.342839386	-1.548621111	3.567457256
O	0.039307000	-3.393977243	3.092942223
H	0.728402053	-2.769150200	2.896238208
H	-0.258807019	-3.203881233	3.973354288

S_3/S_2

C	-0.453532033	-0.154929012	0.149492012
N	0.339901025	-0.870863062	1.064731079
C	1.563862114	-0.540722039	1.063107076
C	1.296375091	1.196285088	-0.472297034
N	-0.007883000	0.807277060	-0.588647040
N	2.164351157	0.365463027	0.278754022
H	3.082863222	0.685919047	0.525880036
N	-1.776934127	-0.509800038	0.149955010
H	-1.939645140	-1.476204104	0.364352025
H	-2.263145163	-0.217870015	-0.678847049
H	1.744251124	1.714164122	-1.302424095
O	2.374075171	-1.189122086	1.927093140
O	-2.877022205	0.341478026	-2.775209201
H	-2.509197179	-0.185885013	-3.470803249
H	-2.483826178	1.206212088	-2.849347203
O	-1.322268093	2.740156198	-2.387010174
H	-1.646955119	3.497289252	-1.918319138
H	-0.915653068	2.163942156	-1.742521127
O	4.848234350	0.979889069	1.367069097
H	5.159503372	1.828059132	1.653637119
H	5.144977372	0.335248022	2.004852144
O	-2.101983152	-3.705726265	0.703559049
H	-2.692433194	-4.443897322	0.635284045
H	-1.585209114	-3.822545276	1.494898105
O	5.341027382	-1.208635085	3.226109233
H	4.500636326	-1.615186116	3.399631242
H	5.955079428	-1.912484139	3.054979222
O	-0.318213023	-3.118109226	2.948320213
H	-0.156303010	-2.360325173	2.393929171
H	-0.725879052	-2.790840202	3.739528272

 S_3/T_1

C	-0.430164032	-0.196040014	0.077325004
N	0.326140024	-0.941340068	1.007654073
C	1.571964114	-0.399142026	1.105214080
C	1.321830093	1.235544086	-0.529380040
N	-0.043483003	0.870551064	-0.571170041
N	2.100636153	0.492613038	0.394829031
H	3.071342224	0.719761054	0.520771036
N	-1.688829121	-0.578837041	-0.012463003
H	-1.933234137	-1.469490104	0.369085028
H	-2.191089155	-0.282529019	-0.826805060
H	1.777014128	1.197064084	-1.510877110
O	2.368290169	-1.007729074	2.110249149
O	-2.910480209	0.300721022	-2.801117200

H	-2.565926187	-0.202793015	-3.525691254
H	-2.518721179	1.168283086	-2.859337207
O	-1.368896097	2.699224195	-2.436533174
H	-1.660900119	3.490208252	-2.003688145
H	-0.933113065	2.163877157	-1.773440128
O	4.800293347	0.828271061	1.474959109
H	5.150951370	1.665096119	1.749766125
H	5.137626369	0.165070011	2.072490151
O	-2.149127156	-3.703612266	0.692306047
H	-2.748668199	-4.437117318	0.665818049
H	-1.589980113	-3.815844272	1.455418106
O	5.431369390	-1.390438098	3.256726233
H	4.624096331	-1.808748131	3.530087256
H	6.044473436	-2.085931148	3.051262217
O	-0.274144020	-3.089965220	2.857397206
H	-0.135390010	-2.353582168	2.261836163
H	-0.697370052	-2.739822197	3.629820260

T_3/T_1

C	-0.492690033	-0.135399011	0.131961010
N	0.311670022	-0.877669064	1.013923072
C	1.514768108	-0.576267039	0.965913069
C	1.267940090	1.161266085	-0.514417035
N	-0.039434003	0.841929063	-0.592081041
N	2.178979156	0.260960019	0.136045009
H	3.016497219	0.677816047	0.503149036
N	-1.828654133	-0.455870034	0.163665014
H	-1.994734143	-1.425815100	0.360957025
H	-2.315097166	-0.160073012	-0.663685046
H	1.702393124	1.780512127	-1.278818090
O	2.404168174	-1.189241088	1.816293130
O	-2.876669206	0.366489028	-2.793546203
H	-2.438184175	-0.160247010	-3.447495250
H	-2.502414180	1.240560089	-2.852054204
O	-1.369485098	2.808267200	-2.351840170
H	-1.725711124	3.544274255	-1.872426136
H	-0.962264069	2.227367161	-1.711981123
O	4.800363346	0.824315059	1.468416107
H	5.055290364	1.662047122	1.831689134
H	5.131086368	0.150162009	2.057547149
O	-2.036092144	-3.731330268	0.737565054
H	-2.610279189	-4.481814322	0.661633050
H	-1.454601104	-3.891113280	1.473188106
O	5.359287384	-1.466089103	3.157020227
H	4.522893325	-1.848461132	3.393620244
H	5.921440425	-2.182766155	2.887996208
O	-0.111803008	-3.053279219	2.934099210

H	-0.164711012	-2.311775166	2.336617169
H	-0.561318041	-2.792926203	3.727816267

Relaxation pathway I

LIIC path connecting Franck-Condon point and $S_2/S_1/T_2$

Coord_1

C	-0.357476028	-0.325875023	0.229680018
N	0.341885027	-0.973917071	1.110492078
C	1.653274120	-0.646333049	1.306678092
C	1.358668096	1.022653073	-0.350634025
N	0.124605007	0.729787053	-0.539943037
N	2.151526155	0.392262029	0.530966037
H	3.102758223	0.691790052	0.672735046
N	-1.649147119	-0.620508046	0.029419001
H	-1.963775141	-1.512845109	0.364878027
H	-2.065503149	-0.287993023	-0.820383060
H	1.807123128	1.824952131	-0.918745067
O	2.363013171	-1.219113085	2.093251151
O	-2.733839197	0.356619025	-2.728166195
H	-2.629401188	-0.143525009	-3.525973252
H	-2.360519169	1.219526087	-2.880668210
O	-1.191319087	2.765921198	-2.329191167
H	-1.566105111	3.489871251	-1.844840131
H	-0.810044059	2.169065158	-1.692877120
O	4.862872351	1.248671090	1.181207087
H	5.136525369	2.113660152	1.453307107
H	5.132414370	0.636409044	1.865785136
O	-2.145668152	-3.642177264	0.683196049
H	-2.886480206	-4.220391304	0.804450057
H	-1.559679111	-3.776041274	1.425256104
O	5.025804364	-0.758670055	3.159791227
H	4.140683299	-1.031827075	2.927287212
H	5.552154399	-1.544063112	3.226183233
O	-0.264665017	-3.327435241	2.832781203
H	-0.002365999	-2.522987184	2.391665171
H	0.533658036	-3.727547270	3.149010225

Coord_2

C	-0.367468027	-0.318725023	0.203398012
N	0.342428026	-0.983659071	1.077050076
C	1.645885117	-0.644421047	1.299170094
C	1.373184100	1.007115075	-0.380227030
N	0.118268009	0.731450051	-0.551278040
N	2.149752157	0.403012026	0.543985041
H	3.103131224	0.691542048	0.691423052
N	-1.661793122	-0.614063042	0.022678002
H	-1.968213139	-1.509167111	0.358436024

H	-2.090763150	-0.280506022	-0.820693058
H	1.817550132	1.809403131	-0.950716067
O	2.343894171	-1.219809086	2.097031148
O	-2.750549197	0.360874028	-2.733004198
H	-2.620789188	-0.139364009	-3.526904255
H	-2.377094170	1.225430086	-2.876265206
O	-1.209606088	2.770026200	-2.326991165
H	-1.577448116	3.497763252	-1.842944131
H	-0.819960057	2.177300156	-1.691718122
O	4.874454352	1.241224090	1.191836088
H	5.143553372	2.107498153	1.464516108
H	5.141549372	0.630519047	1.878381136
O	-2.113412153	-3.632328259	0.700916052
H	-2.843952204	-4.223411303	0.822641060
H	-1.521841112	-3.759403270	1.439642105
O	5.022761362	-0.771654054	3.172112230
H	4.135657300	-1.038289076	2.940743210
H	5.545177398	-1.560446111	3.229925231
O	-0.220476017	-3.337566239	2.849152206
H	0.081686007	-2.546657182	2.431354174
H	0.544505037	-3.769535273	3.177120231

Coord_3

C	-0.377294028	-0.311339021	0.177293011
N	0.343430023	-0.993124073	1.043369077
C	1.638426120	-0.642561047	1.291784092
C	1.387779099	0.989598069	-0.409009028
N	0.112510010	0.733068052	-0.562421042
N	2.146672155	0.413700031	0.557036039
H	3.101849223	0.692198048	0.709649049
N	-1.673956118	-0.607638042	0.016482003
H	-1.971901139	-1.505593111	0.352385025
H	-2.115670152	-0.273049020	-0.820128061
H	1.829645134	1.791414131	-0.981254071
O	2.324231167	-1.220891089	2.100762150
O	-2.766123201	0.364844027	-2.737226196
H	-2.611425191	-0.135300007	-3.526608254
H	-2.392525174	1.230918088	-2.871254204
O	-1.226999091	2.774044201	-2.324598167
H	-1.587659115	3.505689253	-1.841004130
H	-0.828627060	2.185689155	-1.690489123
O	4.884310353	1.234536088	1.201996085
H	5.148801371	2.101986152	1.475574108
H	5.149054370	0.625177045	1.890262134
O	-2.080719149	-3.621743259	0.718489050
H	-2.800739203	-4.225511306	0.840824061
H	-1.483452107	-3.742080271	1.453659105

O	5.018397359	-0.784648054	3.183015229
H	4.129375299	-1.044796077	2.952774214
H	5.536968398	-1.576680116	3.231781230
O	-0.176288013	-3.347696242	2.865522204
H	0.165737013	-2.570326185	2.471042177
H	0.555352039	-3.811522275	3.205228232

Coord_4

C	-0.386954026	-0.303783021	0.151326013
N	0.344880027	-1.002410070	1.009379075
C	1.630863119	-0.640894044	1.284493093
C	1.402475103	0.969880068	-0.436982031
N	0.107371006	0.734555051	-0.573406042
N	2.142243153	0.424194029	0.570077041
H	3.098904225	0.693644051	0.727364051
N	-1.685645120	-0.601228044	0.010842000
H	-1.974882143	-1.502107108	0.346716023
H	-2.140240154	-0.265579017	-0.818643057
H	1.843446135	1.770806128	-1.010317073
O	2.303963165	-1.222572089	2.104373149
O	-2.780587202	0.368625025	-2.740708199
H	-2.601430186	-0.131262009	-3.524995253
H	-2.406800175	1.236066088	-2.865535206
O	-1.243383091	2.777992202	-2.321967167
H	-1.596531115	3.513696256	-1.838968131
H	-0.835909063	2.194237157	-1.689190120
O	4.892375353	1.228696088	1.211633085
H	5.152118370	2.097252149	1.486386109
H	5.154904372	0.620533044	1.901418138
O	-2.047693149	-3.610441260	0.735839052
H	-2.756971197	-4.226682306	0.858926061
H	-1.444594103	-3.724131267	1.467203106
O	5.012797362	-0.797443057	3.192560232
H	4.121949297	-1.051240075	2.963451211
H	5.527686396	-1.592496112	3.231869232
O	-0.132099009	-3.357827240	2.881892207
H	0.249789019	-2.593994187	2.510731179
H	0.566199040	-3.853508278	3.233337234

Coord_5

C	-0.396448027	-0.296129023	0.125449008
N	0.346759024	-1.011632073	0.974999069
C	1.623152118	-0.639576048	1.277273094
C	1.417290102	0.947710071	-0.464128035
N	0.102904009	0.735814054	-0.584265040
N	2.136398152	0.434355031	0.583070041
H	3.094257223	0.695769052	0.744525052

N	-1.696864122	-0.594824042	0.005775001
H	-1.977205141	-1.498686110	0.341427024
H	-2.164495157	-0.258037019	-0.816176059
H	1.859007132	1.747367126	-1.037814076
O	2.283020166	-1.225076087	2.107794153
O	-2.793946203	0.372314026	-2.743331198
H	-2.590898188	-0.127173009	-3.521990252
H	-2.419882172	1.240954088	-2.859005206
O	-1.258624089	2.781889201	-2.319042166
H	-1.603834116	3.521827254	-1.836769130
H	-0.841649059	2.202945160	-1.687814122
O	4.898555355	1.223811089	1.220679090
H	5.153323370	2.093439151	1.496836106
H	5.159064372	0.616756047	1.911818138
O	-2.014459145	-3.598444257	0.752886053
H	-2.712799195	-4.226914303	0.876873065
H	-1.405361103	-3.705627267	1.480155106
O	5.006068360	-0.809815057	3.200795230
H	4.113504295	-1.057503078	2.972839213
H	5.517518398	-1.607607118	3.230282235
O	-0.087911005	-3.367957243	2.898261210
H	0.333840024	-2.617663190	2.550419182
H	0.577047041	-3.895495281	3.261446235

Coord_6

C	-0.405773030	-0.288458022	0.099605007
N	0.349053024	-1.020919076	0.940130067
C	1.615237118	-0.638775048	1.270103091
C	1.432226104	0.922806068	-0.490410036
N	0.099168007	0.736736055	-0.595034040
N	2.129054151	0.444028031	0.595979045
H	3.087845225	0.698465052	0.761090057
N	-1.707619125	-0.588411043	0.001307999
H	-1.978924142	-1.495302106	0.336523022
H	-2.188461155	-0.250344020	-0.812638059
H	1.876397135	1.720851123	-1.063604079
O	2.261312162	-1.228643086	2.110956151
O	-2.806183204	0.376013027	-2.744976198
H	-2.579903187	-0.122953011	-3.517527255
H	-2.431712173	1.245664088	-2.851555206
O	-1.272571089	2.785758201	-2.315753166
H	-1.609313116	3.530127257	-1.834326130
H	-0.845666059	2.211812160	-1.686356122
O	4.902736352	1.220008088	1.229052087
H	5.152209373	2.090713153	1.506792110
H	5.161483373	0.614038044	1.921414137
O	-1.981158143	-3.585778256	0.769545055

H	-2.668402192	-4.226193304	0.894595063
H	-1.365849100	-3.686651267	1.492382106
O	4.998325359	-0.821523062	3.207752233
H	4.104177297	-1.063454079	2.980995215
H	5.506666397	-1.621708115	3.227098234
O	-0.043722005	-3.378087246	2.914631208
H	0.417892030	-2.641332188	2.590107185
H	0.587894042	-3.937482283	3.289555236

Coord_7

C	-0.414922028	-0.280857020	0.073732007
N	0.351746028	-1.030411076	0.904660067
C	1.607054117	-0.638674044	1.262962093
C	1.447281107	0.894849063	-0.515774036
N	0.096233005	0.737200054	-0.605753044
N	2.120103155	0.453042031	0.608764041
H	3.079576222	0.701622049	0.777009058
N	-1.717911126	-0.581963039	-0.002517000
H	-1.980097142	-1.491921108	0.332019025
H	-2.212166158	-0.242398016	-0.807917057
H	1.895704135	1.690970119	-1.087492077
O	2.238740159	-1.233532091	2.113788155
O	-2.817265203	0.379830025	-2.745522198
H	-2.568500184	-0.118513007	-3.511550251
H	-2.442212177	1.250287092	-2.843071203
O	-1.285047094	2.789623200	-2.312015169
H	-1.612686119	3.538635257	-1.831542134
H	-0.847753060	2.220834161	-1.684804119
O	4.904774351	1.217433090	1.236649088
H	5.148535369	2.089259149	1.516093109
H	5.162095372	0.612594046	1.930139138
O	-1.947944142	-3.572474259	0.785727057
H	-2.623981191	-4.224506303	0.912020066
H	-1.326161097	-3.667305266	1.503731111
O	4.989697357	-0.832300058	3.213452229
H	4.094112293	-1.068950076	2.987971216
H	5.495351396	-1.634466118	3.222385233
O	0.000466999	-3.388217244	2.931001210
H	0.501943036	-2.665001191	2.629796187
H	0.598741043	-3.979469286	3.317663237

Coord_8

C	-0.423886032	-0.273419021	0.047755003
N	0.354824024	-1.040264076	0.868456062
C	1.598526113	-0.639475044	1.255826090
C	1.462438103	0.863475065	-0.540152041
N	0.094186004	0.737069050	-0.616470042

N	2.109416150	0.461204034	0.621373044
H	3.069326222	0.705127049	0.792220057
N	-1.727731126	-0.575447042	-0.005641998
H	-1.980784142	-1.488500109	0.327939026
H	-2.235636159	-0.234070015	-0.801862058
H	1.917037138	1.657388118	-1.109223079
O	2.215183162	-1.240025090	2.116213152
O	-2.827139206	0.383884026	-2.744838199
H	-2.556731182	-0.113753010	-3.504006253
H	-2.451281174	1.254925092	-2.833426202
O	-1.295854095	2.793513203	-2.307728166
H	-1.613631118	3.547392257	-1.828303130
H	-0.847672059	2.230003162	-1.683145122
O	4.904496353	1.216252088	1.243342090
H	5.142020372	2.089280152	1.524552108
H	5.160808371	0.612666046	1.937904142
O	-1.914983136	-3.558572254	0.801331060
H	-2.579754186	-4.221844303	0.929070067
H	-1.286392093	-3.647712262	1.514022111
O	4.980312361	-0.841848061	3.217911230
H	4.083453293	-1.073825080	2.993818217
H	5.483805394	-1.645518117	3.216208232
O	0.044655003	-3.398347247	2.947371213
H	0.585995042	-2.688670194	2.669484190
H	0.609588044	-4.021456288	3.345772243

Coord_9

C	-0.432648032	-0.266241018	0.021596004
N	0.358279028	-1.050646074	0.831365060
C	1.589566116	-0.641397048	1.248668090
C	1.477665104	0.828263060	-0.563457039
N	0.093124009	0.736194051	-0.627235047
N	2.096844153	0.468292036	0.633738043
H	3.056943221	0.708859051	0.806640057
N	-1.737061124	-0.568819039	-0.007996001
H	-1.981043142	-1.484988108	0.324315024
H	-2.258893160	-0.225201015	-0.794288055
H	1.940528141	1.619700114	-1.128472082
O	2.190504155	-1.248428092	2.118145151
O	-2.835737203	0.388311027	-2.742778197
H	-2.544627184	-0.108553008	-3.494838252
H	-2.458800180	1.259690090	-2.822473201
O	-1.304758095	2.797460199	-2.302768167
H	-1.611785115	3.556437256	-1.824464129
H	-0.845148058	2.239304161	-1.681362123
O	4.901694355	1.216645087	1.248974092
H	5.132345371	2.091003153	1.531932109

H	5.157508374	0.614526046	1.944597139
O	-1.882446133	-3.544116253	0.816239058
H	-2.535959181	-4.218199304	0.945656069
H	-1.246636091	-3.628015263	1.523043112
O	4.970293358	-0.849830060	3.221141233
H	4.072343296	-1.077886076	2.998584215
H	5.472259392	-1.654457116	3.208638229
O	0.088844008	-3.408478244	2.963741211
H	0.670047048	-2.712339197	2.709172193
H	0.620435046	-4.063443291	3.373881244

Coord_10

C	-0.451273034	-0.206392013	0.003103000
N	0.335008024	-1.025556076	0.800971056
C	1.561200115	-0.634017047	1.249789088
C	1.504268109	0.801837060	-0.576528040
N	0.103719005	0.776500058	-0.629494047
N	2.086553148	0.474402033	0.654833049
H	3.051260222	0.693035047	0.829636058
N	-1.761930126	-0.481940035	-0.002097002
H	-2.016053144	-1.396358100	0.328027023
H	-2.290486164	-0.124101008	-0.777553057
H	1.994073142	1.580866114	-1.135219081
O	2.132567152	-1.260817089	2.127673152
O	-2.838203206	0.497246038	-2.731611197
H	-2.537536182	-0.004727003	-3.476592252
H	-2.441886177	1.360718096	-2.801908204
O	-1.257381088	2.873063207	-2.287704162
H	-1.536893109	3.643065260	-1.810262128
H	-0.797474057	2.310325167	-1.670300122
O	4.915076353	1.160494084	1.263647092
H	5.156067371	2.031405147	1.548772112
H	5.158310374	0.554636041	1.960138143
O	-1.928169138	-3.446720249	0.836115061
H	-2.584562185	-4.117765299	0.966918067
H	-1.286629091	-3.539599254	1.536491109
O	4.935176357	-0.916059064	3.232391234
H	4.031943290	-1.122353083	3.011176215
H	5.419615390	-1.731207127	3.208732232
O	0.132418007	-3.422491244	2.982061216
H	0.753433053	-2.739870199	2.750735197
H	0.630725045	-4.109244296	3.403984244

LIIC path connecting S₂/S₁/T₂ and S1-MIN

Coord_1

C	-0.451273034	-0.206392013	0.003103000
N	0.335008024	-1.025556076	0.800971056

C	1.561200115	-0.634017047	1.249789088
C	1.504268109	0.801837060	-0.576528040
N	0.103719005	0.776500058	-0.629494047
N	2.086553148	0.474402033	0.654833049
H	3.051260222	0.693035047	0.829636058
N	-1.761930126	-0.481940035	-0.002097002
H	-2.016053144	-1.396358100	0.328027023
H	-2.290486164	-0.124101008	-0.777553057
H	1.994073142	1.580866114	-1.135219081
O	2.132567152	-1.260817089	2.127673152
O	-2.838203206	0.497246038	-2.731611197
H	-2.537536182	-0.004727003	-3.476592252
H	-2.441886177	1.360718096	-2.801908204
O	-1.257381088	2.873063207	-2.287704162
H	-1.536893109	3.643065260	-1.810262128
H	-0.797474057	2.310325167	-1.670300122
O	4.915076353	1.160494084	1.263647092
H	5.156067371	2.031405147	1.548772112
H	5.158310374	0.554636041	1.960138143
O	-1.928169138	-3.446720249	0.836115061
H	-2.584562185	-4.117765299	0.966918067
H	-1.286629091	-3.539599254	1.536491109
O	4.935176357	-0.916059064	3.232391234
H	4.031943290	-1.122353083	3.011176215
H	5.419615390	-1.731207127	3.208732232
O	0.132418007	-3.422491244	2.982061216
H	0.753433053	-2.739870199	2.750735197
H	0.630725045	-4.109244296	3.403984244

Coord_2

C	-0.459124035	-0.205068016	0.007981998
N	0.327128025	-1.012968071	0.811189061
C	1.561595114	-0.635502045	1.249967087
C	1.501912106	0.809239059	-0.578049043
N	0.102637007	0.773345056	-0.626459046
N	2.091878153	0.464292032	0.645509046
H	3.057204222	0.681297049	0.819211060
N	-1.771699130	-0.478050032	-0.001329002
H	-2.024570146	-1.393166102	0.327992023
H	-2.291573163	-0.132169008	-0.788157055
H	1.981371142	1.605507115	-1.121314081
O	2.131996154	-1.263934091	2.126068152
O	-2.831846205	0.495555036	-2.740924198
H	-2.533392184	-0.002810000	-3.489150252
H	-2.439121173	1.360434098	-2.810553203
O	-1.260916093	2.878279207	-2.291249163
H	-1.547008110	3.647332265	-1.816123131

H	-0.803535057	2.317993168	-1.670325121
O	4.918670355	1.153091085	1.263044089
H	5.157595370	2.023572144	1.551234114
H	5.157644372	0.546110037	1.960065143
O	-1.917303139	-3.447941246	0.841302062
H	-2.572281188	-4.120306297	0.972198071
H	-1.277449093	-3.537298254	1.543760110
O	4.928511354	-0.923900068	3.229851231
H	4.025633291	-1.128019079	3.004531215
H	5.411568387	-1.739837124	3.205960233
O	0.141701009	-3.416677248	2.988170213
H	0.766108054	-2.735388195	2.760967199
H	0.636814045	-4.108406296	3.405629244

Coord_3

C	-0.466831035	-0.203505012	0.013000001
N	0.319540025	-1.000141074	0.821264061
C	1.562013111	-0.636974047	1.250264088
C	1.499462106	0.816631056	-0.579188039
N	0.101539007	0.770381055	-0.623181047
N	2.096931150	0.454208031	0.636313046
H	3.062876219	0.669583049	0.808843059
N	-1.781297130	-0.473822033	-0.000408001
H	-2.032871148	-1.389702097	0.327863026
H	-2.291966167	-0.139514010	-0.798333059
H	1.968644143	1.629603116	-1.106571081
O	2.131397152	-1.267091089	2.124599150
O	-2.824946205	0.493274033	-2.750076197
H	-2.528504185	-0.001685001	-3.501317254
H	-2.435988174	1.359693096	-2.819127203
O	-1.264590091	2.883463207	-2.294598167
H	-1.557468113	3.651597264	-1.822056129
H	-0.809812057	2.325804168	-1.669968122
O	4.921879355	1.145762080	1.262674088
H	5.158630372	2.015791143	1.554016110
H	5.156638369	0.537606037	1.960149139
O	-1.906212140	-3.448752247	0.846299061
H	-2.559833182	-4.122379296	0.977262069
H	-1.268111094	-3.534679255	1.550832114
O	4.921670357	-0.931857069	3.227306232
H	4.019188288	-1.133865080	2.997875218
H	5.403431387	-1.748525125	3.203100231
O	0.151006009	-3.410754246	2.994190218
H	0.778858056	-2.730927199	2.771120200
H	0.642790049	-4.107384296	3.407347244

Coord_4

C	-0.474394037	-0.201713017	0.018150002
N	0.312247021	-0.987083070	0.831187061
C	1.562456112	-0.638434047	1.250675090
C	1.496927109	0.824010057	-0.579955039
N	0.100427010	0.767600054	-0.619669046
N	2.101717151	0.444152033	0.627241043
H	3.068279219	0.657896048	0.798533057
N	-1.790731127	-0.469274035	0.000672002
H	-2.040959146	-1.385984098	0.327655022
H	-2.291690164	-0.146164011	-0.808073059
H	1.955915139	1.653147117	-1.091014080
O	2.130771151	-1.270292092	2.123265153
O	-2.817492204	0.490437035	-2.759071199
H	-2.522859181	-0.001315000	-3.513101254
H	-2.432472177	1.358522096	-2.827627202
O	-1.268388091	2.888625210	-2.297745163
H	-1.568251110	3.655862263	-1.828055131
H	-0.816306057	2.333753167	-1.669229121
O	4.924693356	1.138523084	1.262561093
H	5.159147373	2.008081147	1.557152110
H	5.155278373	0.529138037	1.960413141
O	-1.894907136	-3.449171250	0.851125062
H	-2.547230185	-4.124004299	0.982133072
H	-1.258621088	-3.531758255	1.557724113
O	4.914641353	-0.939930070	3.224766234
H	4.012604291	-1.139900082	2.991204214
H	5.395203390	-1.757268128	3.200161228
O	0.160338013	-3.404723245	3.000129217
H	0.791681058	-2.726490195	2.781194201
H	0.648662048	-4.106177296	3.409150247

Coord_5

C	-0.481810033	-0.199704016	0.023423004
N	0.305256023	-0.973801070	0.840946063
C	1.562931112	-0.639885045	1.251196091
C	1.494317106	0.831376062	-0.580362040
N	0.099307006	0.764996057	-0.615932044
N	2.106240150	0.434122029	0.618289047
H	3.073414223	0.646235045	0.788281057
N	-1.800001127	-0.464423036	0.001917998
H	-2.048839146	-1.382027101	0.327383025
H	-2.290764167	-0.152145010	-0.817373058
H	1.943204138	1.676133121	-1.074666080
O	2.130118152	-1.273538092	2.122063153
O	-2.809473200	0.487073034	-2.767903200
H	-2.516444182	-0.001669999	-3.524506251
H	-2.428556176	1.356942099	-2.836046206

O	-1.272293091	2.893768209	-2.300685166
H	-1.579333114	3.660125262	-1.834111131
H	-0.823020062	2.341834169	-1.668110122
O	4.927098355	1.131392082	1.262729091
H	5.159119369	2.000457142	1.560675113
H	5.153553372	0.520719039	1.960878139
O	-1.883399134	-3.449216246	0.855796062
H	-2.534483184	-4.125195297	0.986830070
H	-1.248990089	-3.528549255	1.564451115
O	4.907411353	-0.948119066	3.222240233
H	4.005870288	-1.146130081	2.984515212
H	5.386881390	-1.766059127	3.197152231
O	0.169697010	-3.398589245	3.005991215
H	0.804574060	-2.722077196	2.791186199
H	0.654435049	-4.104785295	3.411049247

Coord_6

C	-0.489075033	-0.197486012	0.028814003
N	0.298574023	-0.960300070	0.850531061
C	1.563442112	-0.641329048	1.251822092
C	1.491643110	0.838728059	-0.580416043
N	0.098184007	0.762563053	-0.611978042
N	2.110504149	0.424119028	0.609452046
H	3.078285220	0.634603047	0.778087055
N	-1.809108130	-0.459281031	0.003335002
H	-2.056512147	-1.377846098	0.327057025
H	-2.289201163	-0.157477011	-0.826226061
H	1.930533137	1.698552123	-1.057551075
O	2.129439154	-1.276834094	2.120994152
O	-2.800880203	0.483207034	-2.776567202
H	-2.509252182	-0.002720998	-3.535533252
H	-2.424227172	1.354972099	-2.844377207
O	-1.276295090	2.898896207	-2.303411165
H	-1.590697116	3.664383266	-1.840220133
H	-0.829956062	2.350037168	-1.666610122
O	4.929083357	1.124384082	1.263206091
H	5.158520372	1.992933141	1.564619113
H	5.151447373	0.512360038	1.961567144
O	-1.871702136	-3.448902248	0.860325063
H	-2.521608180	-4.125967297	0.991367072
H	-1.239227091	-3.525066253	1.571026111
O	4.899969353	-0.956427070	3.219735230
H	3.998981289	-1.152564082	2.977804213
H	5.378464387	-1.774894128	3.194080230
O	0.179083011	-3.392353245	3.011781218
H	0.817532060	-2.717690195	2.801093202
H	0.660113047	-4.103207294	3.413054246

Coord_7

C	-0.496183037	-0.195070017	0.034314001
N	0.292209020	-0.946587066	0.859931064
C	1.563998113	-0.642769046	1.252550092
C	1.488916106	0.846064059	-0.580127043
N	0.097065009	0.760294053	-0.607816042
N	2.114516154	0.414144032	0.600727046
H	3.082897222	0.623000047	0.767951057
N	-1.818051131	-0.453863034	0.004930000
H	-2.063979150	-1.373452101	0.326691025
H	-2.287013163	-0.162174009	-0.834624062
H	1.917925139	1.720400121	-1.039692073
O	2.128734152	-1.280182092	2.120058154
O	-2.791704200	0.478859033	-2.785054199
H	-2.501272178	-0.004447999	-3.546178256
H	-2.419473176	1.352626098	-2.852608205
O	-1.280384090	2.904008207	-2.305918168
H	-1.602326114	3.668629263	-1.846374131
H	-0.837120058	2.358354167	-1.664731119
O	4.930636355	1.117515080	1.264016093
H	5.157323373	1.985523141	1.569017110
H	5.148948371	0.504074038	1.962504142
O	-1.859828134	-3.448243248	0.864722060
H	-2.508620180	-4.126333298	0.995755073
H	-1.229346087	-3.521323255	1.577458112
O	4.892302353	-0.964854069	3.217260231
H	3.991929288	-1.159212083	2.971065215
H	5.369950385	-1.783770129	3.190953232
O	0.188491015	-3.386019242	3.017501217
H	0.830547058	-2.713331198	2.810915203
H	0.665693046	-4.101444298	3.415173247

Coord_8

C	-0.503127038	-0.192461014	0.039920005
N	0.286173018	-0.932667070	0.869135065
C	1.564606111	-0.644208048	1.253377090
C	1.486150107	0.853385062	-0.579503043
N	0.095956007	0.758184053	-0.603454044
N	2.118285150	0.404195029	0.592111045
H	3.087256224	0.611427047	0.757873056
N	-1.826827133	-0.448179030	0.006707999
H	-2.071240150	-1.368853096	0.326294026
H	-2.284203163	-0.166250013	-0.842559059
H	1.905403139	1.741671126	-1.021113072
O	2.128003152	-1.283588094	2.119257154
O	-2.781936202	0.474048034	-2.793350201

H	-2.492497181	-0.006831001	-3.556434256
H	-2.414283175	1.349916097	-2.860730208
O	-1.284554091	2.909105211	-2.308201166
H	-1.614207117	3.672856267	-1.852569135
H	-0.844519062	2.366776171	-1.662473120
O	4.931745357	1.110800080	1.265188093
H	5.155500374	1.978241143	1.573907116
H	5.146043373	0.495870034	1.963713143
O	-1.847792136	-3.447252247	0.868995061
H	-2.495536177	-4.126303299	1.000003070
H	-1.219361089	-3.517331253	1.583757115
O	4.884398350	-0.973406071	3.214823232
H	3.984707289	-1.166085085	2.964295212
H	5.361337385	-1.792685130	3.187780232
O	0.197915016	-3.379590241	3.023151216
H	0.843611063	-2.709001194	2.820647201
H	0.671174047	-4.099496296	3.417411249

Coord_9

C	-0.509895035	-0.189668011	0.045624001
N	0.280478018	-0.918545064	0.878132063
C	1.565276113	-0.645647045	1.254302092
C	1.483358104	0.860690063	-0.578553042
N	0.094868008	0.756229056	-0.598899045
N	2.121818155	0.394274029	0.583601044
H	3.091369222	0.599886045	0.747856053
N	-1.835427131	-0.442237031	0.008675999
H	-2.078295152	-1.364057099	0.325876023
H	-2.280772163	-0.169709012	-0.850019061
H	1.892989138	1.762360125	-1.001838071
O	2.127246153	-1.287056094	2.118592153
O	-2.771569202	0.468786033	-2.801443200
H	-2.482921179	-0.009859001	-3.566292257
H	-2.408648173	1.346850096	-2.868729209
O	-1.288800093	2.914184212	-2.310254167
H	-1.626330118	3.677056262	-1.858801134
H	-0.852159059	2.375291173	-1.659836119
O	4.932397356	1.104253078	1.266750092
H	5.153024369	1.971098139	1.579325113
H	5.142717372	0.487759033	1.965220139
O	-1.835609131	-3.445942247	0.873150065
H	-2.482377180	-4.125886296	1.004115074
H	-1.209287089	-3.513102254	1.589930116
O	4.876246353	-0.982085070	3.212433229
H	3.977310285	-1.173194084	2.957487214
H	5.352625387	-1.801637132	3.184569227
O	0.207347013	-3.373069243	3.028733216

H	0.856711063	-2.704703196	2.830288202
H	0.676549049	-4.097365294	3.419776247

Coord_10

C	-0.528514036	-0.198852015	0.053044002
N	0.272746019	-0.910152065	0.884654066
C	1.562816111	-0.642046047	1.248051090
C	1.456630102	0.873824062	-0.582809040
N	0.070876006	0.748146053	-0.594151045
N	2.110098154	0.394877027	0.566599039
H	3.079049219	0.607218045	0.725546052
N	-1.853804134	-0.459780034	0.017630000
H	-2.085728150	-1.385158100	0.332370023
H	-2.292495164	-0.199327015	-0.848195061
H	1.847113132	1.792133130	-0.988200073
O	2.132379151	-1.281374091	2.107923151
O	-2.789862203	0.433758029	-2.797952202
H	-2.500767179	-0.039636000	-3.565975258
H	-2.439824174	1.317267093	-2.865880208
O	-1.341935098	2.902234209	-2.304437165
H	-1.692337122	3.660765265	-1.855336134
H	-0.901531063	2.370124170	-1.651441118
O	4.913998355	1.132336081	1.249375092
H	5.124980367	2.000144144	1.565857113
H	5.128620371	0.515414037	1.946282139
O	-1.803395127	-3.468521251	0.881142065
H	-2.442738174	-4.155033300	1.014047074
H	-1.175779083	-3.528008256	1.597332115
O	4.875443353	-0.958641068	3.189077229
H	3.977989288	-1.155925083	2.933095212
H	5.358459386	-1.774142130	3.157625225
O	0.244686019	-3.374689245	3.029956218
H	0.891092063	-2.702802195	2.833502202
H	0.717654050	-4.099522294	3.415423246

LIIC path connecting S1-MIN and S₁/T₁/S₀-II

Coord_1

C	-0.528514036	-0.198852015	0.053044002
N	0.272746019	-0.910152065	0.884654066
C	1.562816111	-0.642046047	1.248051090
C	1.456630102	0.873824062	-0.582809040
N	0.070876006	0.748146053	-0.594151045
N	2.110098154	0.394877027	0.566599039
H	3.079049219	0.607218045	0.725546052
N	-1.853804134	-0.459780034	0.017630000
H	-2.085728150	-1.385158100	0.332370023
H	-2.292495164	-0.199327015	-0.848195061

H	1.847113132	1.792133130	-0.988200073
O	2.132379151	-1.281374091	2.107923151
O	-2.789862203	0.433758029	-2.797952202
H	-2.500767179	-0.039636000	-3.565975258
H	-2.439824174	1.317267093	-2.865880208
O	-1.341935098	2.902234209	-2.304437165
H	-1.692337122	3.660765265	-1.855336134
H	-0.901531063	2.370124170	-1.651441118
O	4.913998355	1.132336081	1.249375092
H	5.124980367	2.000144144	1.565857113
H	5.128620371	0.515414037	1.946282139
O	-1.803395127	-3.468521251	0.881142065
H	-2.442738174	-4.155033300	1.014047074
H	-1.175779083	-3.528008256	1.597332115
O	4.875443353	-0.958641068	3.189077229
H	3.977989288	-1.155925083	2.933095212
H	5.358459386	-1.774142130	3.157625225
O	0.244686019	-3.374689245	3.029956218
H	0.891092063	-2.702802195	2.833502202
H	0.717654050	-4.099522294	3.415423246

Coord_2

C	-0.533043037	-0.209228016	0.066405003
N	0.270119019	-0.919401067	0.889552062
C	1.559135112	-0.628649046	1.249666091
C	1.450239107	0.861553061	-0.588429040
N	0.053057004	0.769748053	-0.558260042
N	2.101852149	0.421119032	0.576653042
H	3.072243222	0.628956043	0.732728051
N	-1.856585135	-0.478082037	0.023529004
H	-2.084503152	-1.405450100	0.334892023
H	-2.296033164	-0.216131017	-0.841502059
H	1.859160133	1.735344124	-1.066178077
O	2.137351153	-1.264086092	2.106140152
O	-2.763214197	0.432924030	-2.795353200
H	-2.488030179	-0.034937002	-3.572260259
H	-2.416378172	1.317558093	-2.861852206
O	-1.342985097	2.921795209	-2.301821167
H	-1.713501121	3.693669269	-1.893545134
H	-0.909048063	2.425084175	-1.617547114
O	4.918280352	1.130715084	1.251013091
H	5.135072370	1.996293141	1.569708115
H	5.133192372	0.510437035	1.944771143
O	-1.809182130	-3.488329250	0.878680063
H	-2.440850175	-4.181146303	1.016354075
H	-1.178947087	-3.540702255	1.592672117
O	4.882587352	-0.966176071	3.187220230

H	3.983822287	-1.159428083	2.933388213
H	5.362199388	-1.783594130	3.153093229
O	0.236425018	-3.379544245	3.031412218
H	0.860606061	-2.689165192	2.830991203
H	0.732885052	-4.086517292	3.422040248

Coord_3

C	-0.537038039	-0.220275015	0.078766007
N	0.267812018	-0.930095067	0.893379067
C	1.555500114	-0.616763042	1.250627088
C	1.442581102	0.846064059	-0.593278045
N	0.036557004	0.789979055	-0.520817037
N	2.092819152	0.446289031	0.586243041
H	3.064621223	0.650255046	0.738715051
N	-1.858648133	-0.496556038	0.028265003
H	-2.082933152	-1.425649103	0.336600022
H	-2.298511163	-0.232617016	-0.835912058
H	1.866165133	1.669336120	-1.141558085
O	2.142501153	-1.248465092	2.103264153
O	-2.735255196	0.433999032	-2.792766201
H	-2.474005178	-0.027358003	-3.578654255
H	-2.391211174	1.319745093	-2.856828208
O	-1.341029099	2.940925210	-2.295612166
H	-1.729288124	3.724406270	-1.928068139
H	-0.916061064	2.478823178	-1.582259115
O	4.920967355	1.131155079	1.250588088
H	5.142630370	1.995061143	1.570502114
H	5.136896369	0.508515036	1.941834140
O	-1.816360129	-3.507914253	0.876441061
H	-2.441667177	-4.205524302	1.019541072
H	-1.183742084	-3.553147256	1.588607115
O	4.890662353	-0.969636070	3.185499229
H	3.990800288	-1.160148081	2.934117213
H	5.367785389	-1.788447130	3.149537227
O	0.227231018	-3.384186241	3.032930221
H	0.831876060	-2.679261195	2.825589203
H	0.744272052	-4.073884291	3.428869248

Coord_4

C	-0.540446041	-0.232015018	0.090215005
N	0.265899021	-0.942164065	0.896306062
C	1.552069114	-0.606321042	1.251056092
C	1.433654105	0.827009058	-0.597309042
N	0.021555003	0.808676056	-0.481742033
N	2.083082153	0.470320033	0.595263042
H	3.056278220	0.671076049	0.743287052
N	-1.860010134	-0.515172039	0.031902001

H	-2.081108152	-1.445779106	0.337448024
H	-2.299956166	-0.248760018	-0.831363060
H	1.867899135	1.593752114	-1.213884089
O	2.147845156	-1.234348088	2.099595150
O	-2.706063197	0.436915032	-2.790104201
H	-2.458776176	-0.016954003	-3.585059258
H	-2.364424169	1.323756098	-2.850763207
O	-1.336210094	2.959711214	-2.285803162
H	-1.739739126	3.753303269	-1.958743142
H	-0.922501067	2.531273184	-1.545499113
O	4.922258352	1.133506081	1.247920092
H	5.147940373	1.996339143	1.567962111
H	5.139864371	0.509558034	1.937381140
O	-1.824912131	-3.527363253	0.874106061
H	-2.444955178	-4.228553303	1.023063075
H	-1.190169085	-3.565465258	1.584783116
O	4.899635352	-0.968914071	3.184007230
H	3.998867289	-1.157915086	2.935372209
H	5.375107387	-1.788662129	3.147162227
O	0.216884015	-3.388595245	3.034312220
H	0.804074056	-2.672188191	2.817539205
H	0.752285055	-4.061399291	3.435750246

Coord_5

C	-0.543192037	-0.244494018	0.100807006
N	0.264475021	-0.955595071	0.898441065
C	1.548998113	-0.597304041	1.251005090
C	1.423416102	0.804057059	-0.600442041
N	0.008232003	0.825674060	-0.440963031
N	2.072696149	0.493147036	0.603578041
H	3.047272221	0.691400048	0.746197056
N	-1.860659133	-0.533927038	0.034491000
H	-2.079087150	-1.465877104	0.337420025
H	-2.300360167	-0.264549021	-0.827799062
H	1.864060134	1.508293111	-1.282575090
O	2.153443152	-1.221647087	2.095315148
O	-2.675662192	0.441609030	-2.787283200
H	-2.442376174	-0.003763001	-3.591373258
H	-2.336049166	1.329519097	-2.843604206
O	-1.328580093	2.978193216	-2.272358165
H	-1.744810126	3.780630273	-1.985378141
H	-0.928220065	2.582331184	-1.507163111
O	4.922278355	1.137675083	1.242855088
H	5.151178371	2.000062143	1.561855114
H	5.142152370	0.513526038	1.931337137
O	-1.834873130	-3.546750254	0.871471065
H	-2.450603176	-4.250502305	1.026577076

H	-1.198254087	-3.577749256	1.580955116
O	4.909407351	-0.963872070	3.182813231
H	4.007917288	-1.152545085	2.937204210
H	5.384012387	-1.784147131	3.146147228
O	0.205248016	-3.392667243	3.035359219
H	0.776598056	-2.667301191	2.806798204
H	0.757270053	-4.048799290	3.442473247

Coord_6

C	-0.545184041	-0.257793020	0.110598008
N	0.263669020	-0.970434069	0.899861065
C	1.546479113	-0.589730044	1.250476092
C	1.411786103	0.776887056	-0.602552046
N	-0.003229003	0.840788061	-0.398394029
N	2.061709149	0.514699039	0.611020046
H	3.037644217	0.711234051	0.747151052
N	-1.860560135	-0.552858042	0.036097001
H	-2.076922148	-1.486006107	0.336536024
H	-2.299688164	-0.279999023	-0.825145058
H	1.854275134	1.412726102	-1.346926097
O	2.159397153	-1.210341089	2.090535148
O	-2.644006189	0.448018033	-2.784193201
H	-2.424767177	0.012173003	-3.597470258
H	-2.306024168	1.336952095	-2.835260203
O	-1.318077094	2.996351214	-2.255181162
H	-1.744346127	3.806589275	-2.007722142
H	-0.932970066	2.631835192	-1.467087105
O	4.921101353	1.143621082	1.235232089
H	5.152443369	2.006215146	1.551946112
H	5.143766371	0.520443036	1.923617139
O	-1.846383132	-3.566173255	0.868412061
H	-2.458654180	-4.271600305	1.029869072
H	-1.208104087	-3.590111260	1.576937116
O	4.919838356	-0.954308069	3.181966230
H	4.017813289	-1.143807083	2.939626212
H	5.394325390	-1.774728130	3.146654227
O	0.192206014	-3.396208243	3.035823217
H	0.748889055	-2.664082190	2.792990202
H	0.759501054	-4.035726288	3.448743246

Coord_7

C	-0.546299038	-0.272052019	0.119666011
N	0.263678022	-0.986788069	0.900637066
C	1.544768113	-0.583660042	1.249442091
C	1.398636102	0.745183052	-0.603459045
N	-0.012649003	0.853789062	-0.353904023
N	2.050166148	0.534898036	0.617392044

H	3.027424216	0.730612051	0.745797051
N	-1.859661131	-0.572069039	0.036834002
H	-2.074692148	-1.506292106	0.334874026
H	-2.297871166	-0.295172021	-0.823276057
H	1.838100133	1.306919096	-1.406100099
O	2.165860154	-1.200485088	2.085317149
O	-2.610955186	0.456057034	-2.780677200
H	-2.405813175	0.030792004	-3.603166259
H	-2.274162162	1.345933096	-2.825571206
O	-1.304470095	3.014067216	-2.234080161
H	-1.738011124	3.831286278	-2.025423148
H	-0.936356070	2.679532192	-1.425003104
O	4.918762353	1.151386081	1.224865088
H	5.151759371	2.014867146	1.537978113
H	5.144674370	0.530424038	1.914116137
O	-1.859767136	-3.585797259	0.864885063
H	-2.469376178	-4.292093308	1.032846075
H	-1.219968087	-3.602723258	1.572578113
O	4.930764358	-0.939917068	3.181485229
H	4.028408291	-1.131394082	2.942610211
H	5.405868391	-1.760106127	3.148825224
O	0.177616015	-3.398888246	3.035333220
H	0.720275050	-2.662048191	2.775246201
H	0.759219055	-4.021632287	3.454091249

Coord_8

C	-0.546373038	-0.287522018	0.128158009
N	0.264816017	-1.004869072	0.900844064
C	1.544248112	-0.579203041	1.247842092
C	1.383784102	0.708655053	-0.602904044
N	-0.019878004	0.864364061	-0.307281020
N	2.038124148	0.553658042	0.622468044
H	3.016634218	0.749629057	0.741708051
N	-1.857896135	-0.591787040	0.036910002
H	-2.072554150	-1.526982111	0.332625023
H	-2.294804165	-0.310226024	-0.821965057
H	1.814995132	1.190889083	-1.459119103
O	2.173060155	-1.192258086	2.079698149
O	-2.576211186	0.465572033	-2.776470198
H	-2.385214172	0.051964005	-3.608168259
H	-2.240066161	1.356254100	-2.814252205
O	-1.287240094	3.031050218	-2.208679160
H	-1.725150122	3.854668277	-2.037955144
H	-0.937744070	2.724986194	-1.380453100
O	4.915255352	1.161156085	1.211541088
H	5.149058371	2.026229148	1.519666109
H	5.144813369	0.543748039	1.902696138

O	-1.875709135	-3.605928262	0.860967061
H	-2.483430179	-4.312322310	1.035581075
H	-1.234379087	-3.615900258	1.567759113
O	4.942025355	-0.920230065	3.181345230
H	4.039577291	-1.114878079	2.946067210
H	5.418513389	-1.739786128	3.152768225
O	0.161247012	-3.400096246	3.033264216
H	0.689747052	-2.660655190	2.751789197
H	0.756677052	-4.005553290	3.457710250

Coord_9

C	-0.545179040	-0.304681024	0.136358007
N	0.267629018	-1.025078076	0.900590065
C	1.545535113	-0.576551043	1.245603090
C	1.366963097	0.667072050	-0.600495044
N	-0.024841004	0.872040063	-0.258125021
N	2.025660145	0.570895043	0.626021046
H	3.005287219	0.768506058	0.734380052
N	-1.855195135	-0.612509045	0.036736003
H	-2.070835149	-1.548587111	0.330203026
H	-2.290323167	-0.325541022	-0.820789061
H	1.784277128	1.064939077	-1.504814109
O	2.181329158	-1.186067088	2.073704147
O	-2.539177182	0.476246035	-2.771098197
H	-2.362352170	0.075403006	-3.611966259
H	-2.202932158	1.367501101	-2.800759201
O	-1.265317091	3.046667218	-2.178248156
H	-1.704471124	3.876375281	-2.044444149
H	-0.936034066	2.767381198	-1.332607095
O	4.910508352	1.173427086	1.195019084
H	5.144107373	2.040830149	1.496733107
H	5.144097371	0.561010039	1.889178136
O	-1.895640136	-3.627169262	0.856984060
H	-2.502286183	-4.332850312	1.038489073
H	-1.252453088	-3.630240263	1.562412110
O	4.953549354	-0.894501065	3.181422231
H	4.051312294	-1.093634078	2.949789215
H	5.432298392	-1.712932123	3.158474226
O	0.142689010	-3.398578243	3.028430219
H	0.655524048	-2.659163191	2.718913197
H	0.752195053	-3.985584289	3.458065248

Coord_10

C	-0.542679037	-0.313289024	0.155888013
N	0.271979019	-1.056551078	0.892797062
C	1.549357112	-0.594863042	1.246452091
C	1.348649098	0.646652048	-0.561765042

N	-0.026274000	0.894693067	-0.165181011
N	2.014081144	0.581812044	0.660302048
H	2.994884218	0.779150056	0.760245056
N	-1.852298133	-0.619415046	0.041062001
H	-2.072390147	-1.562821112	0.309467020
H	-2.284787163	-0.304507020	-0.807365057
H	1.746071124	0.978772071	-1.500164107
O	2.190152157	-1.222662086	2.055813146
O	-2.498641178	0.572666041	-2.731083195
H	-2.336800169	0.206473014	-3.590335261
H	-2.159778155	1.463796104	-2.729688199
O	-1.232392090	3.126873227	-2.046259147
H	-1.667943119	3.960723288	-1.927594139
H	-0.925171067	2.850878203	-1.191430088
O	4.906577354	1.166705085	1.221135087
H	5.139989368	2.029385145	1.536289112
H	5.143999373	0.543479037	1.904202139
O	-1.927764137	-3.653831265	0.783632055
H	-2.535338181	-4.361271316	0.955511069
H	-1.281447091	-3.668203264	1.486016109
O	4.965363358	-0.932913068	3.176402228
H	4.063382293	-1.131146083	2.943686214
H	5.446320394	-1.749595126	3.140434225
O	0.117196007	-3.450725248	2.952999215
H	0.611185043	-2.708221192	2.620999187
H	0.741587055	-4.028244288	3.372324241

LIIC path connecting S₁/T₁/S₀-II and S₀-MIN

Coord_1

C	-0.542679037	-0.313289024	0.155888013
N	0.271979019	-1.056551078	0.892797062
C	1.549357112	-0.594863042	1.246452091
C	1.348649098	0.646652048	-0.561765042
N	-0.026274000	0.894693067	-0.165181011
N	2.014081144	0.581812044	0.660302048
H	2.994884218	0.779150056	0.760245056
N	-1.852298133	-0.619415046	0.041062001
H	-2.072390147	-1.562821112	0.309467020
H	-2.284787163	-0.304507020	-0.807365057
H	1.746071124	0.978772071	-1.500164107
O	2.190152157	-1.222662086	2.055813146
O	-2.498641178	0.572666041	-2.731083195
H	-2.336800169	0.206473014	-3.590335261
H	-2.159778155	1.463796104	-2.729688199
O	-1.232392090	3.126873227	-2.046259147
H	-1.667943119	3.960723288	-1.927594139
H	-0.925171067	2.850878203	-1.191430088

O	4.906577354	1.166705085	1.221135087
H	5.139989368	2.029385145	1.536289112
H	5.143999373	0.543479037	1.904202139
O	-1.927764137	-3.653831265	0.783632055
H	-2.535338181	-4.361271316	0.955511069
H	-1.281447091	-3.668203264	1.486016109
O	4.965363358	-0.932913068	3.176402228
H	4.063382293	-1.131146083	2.943686214
H	5.446320394	-1.749595126	3.140434225
O	0.117196007	-3.450725248	2.952999215
H	0.611185043	-2.708221192	2.620999187
H	0.741587055	-4.028244288	3.372324241

Coord_2

C	-0.521951037	-0.315171021	0.163903011
N	0.279914021	-1.047836074	0.916799065
C	1.561065111	-0.601019046	1.252952092
C	1.349879096	0.687986051	-0.538498039
N	-0.009387001	0.875898061	-0.207009017
N	2.029488144	0.560325040	0.645737047
H	3.006999218	0.769039056	0.750323057
N	-1.829570134	-0.620049043	0.039589004
H	-2.060145150	-1.557788112	0.315446024
H	-2.260278165	-0.303195021	-0.808990060
H	1.752951126	1.072358078	-1.435757103
O	2.209537158	-1.222688090	2.059779150
O	-2.524652182	0.548122038	-2.730936195
H	-2.369181171	0.167047012	-3.583361260
H	-2.181981158	1.436124103	-2.746642196
O	-1.227759090	3.086264223	-2.077880150
H	-1.656573122	3.907895279	-1.918582139
H	-0.912294068	2.774627201	-1.247331092
O	4.901840355	1.175449083	1.216493086
H	5.139705369	2.038392144	1.526861110
H	5.142847370	0.553448038	1.899727136
O	-1.951749138	-3.653061265	0.772297057
H	-2.574114183	-4.346159311	0.938555066
H	-1.312129094	-3.680696266	1.479088104
O	4.972251356	-0.913911065	3.174352227
H	4.072148294	-1.120490083	2.941663211
H	5.458270391	-1.727105125	3.149756227
O	0.074995005	-3.437506247	2.939459209
H	0.543221042	-2.688114193	2.595334186
H	0.718722052	-3.995295289	3.347327241

Coord_3

C	-0.501223037	-0.317052024	0.171917014
---	--------------	--------------	-------------

N	0.287850018	-1.039121075	0.940800069
C	1.572773115	-0.607174044	1.259451092
C	1.351109095	0.729319054	-0.515232037
N	0.007500003	0.857102061	-0.248836018
N	2.044894145	0.538838041	0.631171047
H	3.019114218	0.758929056	0.740401052
N	-1.806842130	-0.620683045	0.038116002
H	-2.047899147	-1.552755113	0.321426023
H	-2.235768162	-0.301883021	-0.810614057
H	1.759831129	1.165943086	-1.371349098
O	2.228921159	-1.222714089	2.063744148
O	-2.550663186	0.523577040	-2.730787194
H	-2.401561172	0.127620010	-3.576385259
H	-2.204183159	1.408452102	-2.763596199
O	-1.223126090	3.045654219	-2.109501152
H	-1.645203119	3.855066276	-1.909570140
H	-0.899416064	2.698375193	-1.303232095
O	4.897101350	1.184192086	1.211850085
H	5.139419370	2.047399149	1.517433108
H	5.141694372	0.563416038	1.895252138
O	-1.975734145	-3.652289264	0.760963054
H	-2.612889186	-4.331046310	0.921598068
H	-1.342811098	-3.693187267	1.472159105
O	4.979138360	-0.894910066	3.172301226
H	4.080914295	-1.109833078	2.939639214
H	5.470218393	-1.704615124	3.159077229
O	0.032794003	-3.424286245	2.925919209
H	0.475257035	-2.668006193	2.569668184
H	0.695858049	-3.962345285	3.322328241

Coord_4

C	-0.480496032	-0.318934022	0.179931012
N	0.295785020	-1.030407076	0.964802067
C	1.584480114	-0.613330042	1.265951093
C	1.352340099	0.770652057	-0.491965034
N	0.024387001	0.838306061	-0.290664019
N	2.060300146	0.517351037	0.616605046
H	3.031228218	0.748818055	0.730479053
N	-1.784115126	-0.621318047	0.036643000
H	-2.035654144	-1.547721113	0.327405023
H	-2.211259159	-0.300571021	-0.812238060
H	1.766711126	1.259528093	-1.306942094
O	2.248305159	-1.222739087	2.067709151
O	-2.576673184	0.499032037	-2.730639199
H	-2.433941173	0.088194009	-3.569410259
H	-2.226385161	1.380780100	-2.780549202
O	-1.218493085	3.005044215	-2.141121154

H	-1.633833116	3.802237273	-1.900558135
H	-0.886539064	2.622123191	-1.359133099
O	4.892363351	1.192936084	1.207208089
H	5.139133371	2.056405147	1.508005106
H	5.140542369	0.573384039	1.890777135
O	-1.999718146	-3.651518263	0.749628056
H	-2.651664189	-4.315933310	0.904642065
H	-1.373493097	-3.705679269	1.465231106
O	4.986024359	-0.875908063	3.170250230
H	4.089679296	-1.099177078	2.937616212
H	5.482167395	-1.682125122	3.168398226
O	-0.009406999	-3.411067244	2.912379209
H	0.407293028	-2.647898193	2.544002183
H	0.672993046	-3.929395285	3.297330236

Coord_5

C	-0.459768033	-0.320815025	0.187946016
N	0.303720023	-1.021691071	0.988803071
C	1.596188113	-0.619485045	1.272451093
C	1.353570097	0.811986060	-0.468698036
N	0.041274005	0.819511061	-0.332491025
N	2.075707147	0.495864038	0.602040045
H	3.043342217	0.738707055	0.720557053
N	-1.761386127	-0.621952043	0.035170004
H	-2.023408147	-1.542688113	0.333384022
H	-2.186749156	-0.299259021	-0.813863057
H	1.773591129	1.353113100	-1.242535089
O	2.267689165	-1.222765086	2.071674149
O	-2.602683188	0.474488034	-2.730491199
H	-2.466322180	0.048768002	-3.562434258
H	-2.248587163	1.353108099	-2.797503200
O	-1.213860085	2.964435211	-2.172742157
H	-1.622462118	3.749408270	-1.891546135
H	-0.873662065	2.545871184	-1.415034103
O	4.887625352	1.201680087	1.202565088
H	5.138847372	2.065412146	1.498577110
H	5.139388371	0.583353040	1.886301137
O	-2.023703147	-3.650746263	0.738293053
H	-2.690440191	-4.300820309	0.887686061
H	-1.404175101	-3.718170265	1.458302107
O	4.992911357	-0.856906059	3.168199229
H	4.098444297	-1.088520078	2.935592209
H	5.494115397	-1.659634121	3.177719228
O	-0.051608006	-3.397847243	2.898839209
H	0.339328026	-2.627790188	2.518336181
H	0.650128049	-3.896445281	3.272332236

Coord_6

C	-0.439040033	-0.322697023	0.195961014
N	0.311655025	-1.012977073	1.012805074
C	1.607895117	-0.625641044	1.278950094
C	1.354800096	0.853319063	-0.445432034
N	0.058161004	0.800715056	-0.374319025
N	2.091113153	0.474377034	0.587474045
H	3.055457222	0.728596055	0.710634049
N	-1.738659123	-0.622586045	0.033697002
H	-2.011163144	-1.537655108	0.339364026
H	-2.162239158	-0.297947022	-0.815487060
H	1.780471127	1.446698107	-1.178127085
O	2.287073166	-1.222790089	2.075640148
O	-2.628694192	0.449943031	-2.730342198
H	-2.498702181	0.009342000	-3.555459257
H	-2.270789165	1.325436098	-2.814456203
O	-1.209227086	2.923825212	-2.204362159
H	-1.611092115	3.696579267	-1.882534135
H	-0.860784061	2.469619177	-1.470935107
O	4.882886353	1.210423085	1.197923087
H	5.138561367	2.074418150	1.489149108
H	5.138236368	0.593321041	1.881826133
O	-2.047688148	-3.649975262	0.726958050
H	-2.729215199	-4.285707308	0.870729063
H	-1.434856104	-3.730662267	1.451374102
O	4.999798361	-0.837905061	3.166148228
H	4.107210298	-1.077864078	2.933568212
H	5.506064394	-1.637144120	3.187040230
O	-0.093808008	-3.384627242	2.885298209
H	0.271364019	-2.607681188	2.492670180
H	0.627263046	-3.863495276	3.247334236

Coord_7

C	-0.418312028	-0.324579026	0.203975017
N	0.319591022	-1.004262074	1.036806072
C	1.619603116	-0.631796047	1.285450094
C	1.356030099	0.894652066	-0.422165031
N	0.075049008	0.781919055	-0.416146031
N	2.106519154	0.452890030	0.572909039
H	3.067571222	0.718485049	0.700712049
N	-1.715931124	-0.623220047	0.032224000
H	-1.998917146	-1.532622109	0.345343025
H	-2.137729155	-0.296634022	-0.817112057
H	1.787351129	1.540284109	-1.113719080
O	2.306457167	-1.222816088	2.079605151
O	-2.654704190	0.425399029	-2.730194198
H	-2.531082183	-0.030085002	-3.548483257

H	-2.292991167	1.297764091	-2.831410206
O	-1.204594086	2.883215208	-2.235983161
H	-1.599722118	3.643750264	-1.873522136
H	-0.847907061	2.393367175	-1.526837112
O	4.878147353	1.219167088	1.193280086
H	5.138275368	2.083425149	1.479721106
H	5.137082370	0.603290041	1.877351135
O	-2.071672149	-3.649204261	0.715624052
H	-2.767990202	-4.270594308	0.853773060
H	-1.465538108	-3.743154268	1.444445103
O	5.006684359	-0.818903058	3.164097227
H	4.115975299	-1.067207078	2.931544210
H	5.518012396	-1.614654118	3.196360232
O	-0.136009010	-3.371407240	2.871758209
H	0.203400013	-2.587573188	2.467004178
H	0.604399044	-3.830545277	3.222335231

Coord_8

C	-0.397584028	-0.326460023	0.211989015
N	0.327526024	-0.995547069	1.060808076
C	1.631310115	-0.637952046	1.291949095
C	1.357260098	0.935986069	-0.398898028
N	0.091936006	0.763124055	-0.457974032
N	2.121925154	0.431403031	0.558343038
H	3.079685222	0.708374049	0.690790050
N	-1.693202120	-0.623854044	0.030751003
H	-1.986671143	-1.527588109	0.351322024
H	-2.113220152	-0.295322022	-0.818736060
H	1.794231127	1.633869116	-1.049312076
O	2.325841168	-1.222841086	2.083570149
O	-2.680715194	0.400854031	-2.730046198
H	-2.563462184	-0.069511004	-3.541508256
H	-2.315193169	1.270091090	-2.848363203
O	-1.199960086	2.842605204	-2.267603164
H	-1.588352115	3.590921261	-1.864509136
H	-0.835029062	2.317115167	-1.582738116
O	4.873409349	1.227910091	1.188637085
H	5.137989369	2.092431148	1.470293104
H	5.135929372	0.613258042	1.872876137
O	-2.095657150	-3.648432260	0.704289049
H	-2.806765204	-4.255480307	0.836816062
H	-1.496220107	-3.755645270	1.437517104
O	5.013571363	-0.799901059	3.162046226
H	4.124740299	-1.056550078	2.929521213
H	5.529961398	-1.592163117	3.205681229
O	-0.178210011	-3.358188244	2.858218203
H	0.135436011	-2.567465182	2.441338177

H 0.581534041 -3.797595272 3.197337231

Coord_9

C -0.376856028 -0.328342026 0.220004018
N 0.335461027 -0.986832071 1.084809079
C 1.643018119 -0.644108044 1.298449095
C 1.358490096 0.977319072 -0.375632025
N 0.108823010 0.744328055 -0.499801038
N 2.137332155 0.409916027 0.543777038
H 3.091800221 0.698264049 0.680868051
N -1.670475121 -0.624488046 0.029278001
H -1.974426140 -1.522555110 0.357301024
H -2.088710148 -0.294010022 -0.820361057
H 1.801111130 1.727454123 -0.984904071
O 2.345225169 -1.222867090 2.087535153
O -2.706725192 0.376309028 -2.729898198
H -2.595843186 -0.108937005 -3.534533255
H -2.337395171 1.242419088 -2.865317206
O -1.195327086 2.801995200 -2.299224166
H -1.576982112 3.538091253 -1.855497136
H -0.822152058 2.240864160 -1.638639119
O 4.868671350 1.236654089 1.183995084
H 5.137704370 2.101438152 1.460865108
H 5.134777369 0.623227043 1.868400134
O -2.119642151 -3.647661265 0.692954051
H -2.845541207 -4.240367306 0.819860059
H -1.526902110 -3.768137271 1.430588104
O 5.020458361 -0.780899056 3.159995230
H 4.133506295 -1.045894078 2.927497210
H 5.541909400 -1.569673116 3.215002231
O -0.220411013 -3.344968243 2.844677203
H 0.067471004 -2.547357183 2.415672176
H 0.558669038 -3.764645273 3.172339226

Coord_10

C -0.357476028 -0.325875023 0.229680018
N 0.341885027 -0.973917071 1.110492078
C 1.653274120 -0.646333049 1.306678092
C 1.358668096 1.022653073 -0.350634025
N 0.124605007 0.729787053 -0.539943037
N 2.151526155 0.392262029 0.530966037
H 3.102758223 0.691790052 0.672735046
N -1.649147119 -0.620508046 0.029419001
H -1.963775141 -1.512845109 0.364878027
H -2.065503149 -0.287993023 -0.820383060
H 1.807123128 1.824952131 -0.918745067
O 2.363013171 -1.219113085 2.093251151

O	-2.733839197	0.356619025	-2.728166195
H	-2.629401188	-0.143525009	-3.525973252
H	-2.360519169	1.219526087	-2.880668210
O	-1.191319087	2.765921198	-2.329191167
H	-1.566105111	3.489871251	-1.844840131
H	-0.810044059	2.169065158	-1.692877120
O	4.862872351	1.248671090	1.181207087
H	5.136525369	2.113660152	1.453307107
H	5.132414370	0.636409044	1.865785136
O	-2.145668152	-3.642177264	0.683196049
H	-2.886480206	-4.220391304	0.804450057
H	-1.559679111	-3.776041274	1.425256104
O	5.025804364	-0.758670055	3.159791227
H	4.140683299	-1.031827075	2.927287212
H	5.552154399	-1.544063112	3.226183233
O	-0.264665017	-3.327435241	2.832781203
H	-0.002365999	-2.522987184	2.391665171
H	0.533658036	-3.727547270	3.149010225

Relaxation pathway II

LIIC path connecting Franck-Condon point and S2-MIN
Coord_1

C	-0.357476028	-0.325875023	0.229680018
N	0.341885027	-0.973917071	1.110492078
C	1.653274120	-0.646333049	1.306678092
C	1.358668096	1.022653073	-0.350634025
N	0.124605007	0.729787053	-0.539943037
N	2.151526155	0.392262029	0.530966037
H	3.102758223	0.691790052	0.672735046
N	-1.649147119	-0.620508046	0.029419001
H	-1.963775141	-1.512845109	0.364878027
H	-2.065503149	-0.287993023	-0.820383060
H	1.807123128	1.824952131	-0.918745067
O	2.363013171	-1.219113085	2.093251151
O	-2.733839197	0.356619025	-2.728166195
H	-2.629401188	-0.143525009	-3.525973252
H	-2.360519169	1.219526087	-2.880668210
O	-1.191319087	2.765921198	-2.329191167
H	-1.566105111	3.489871251	-1.844840131
H	-0.810044059	2.169065158	-1.692877120
O	4.862872351	1.248671090	1.181207087
H	5.136525369	2.113660152	1.453307107
H	5.132414370	0.636409044	1.865785136
O	-2.145668152	-3.642177264	0.683196049
H	-2.886480206	-4.220391304	0.804450057
H	-1.559679111	-3.776041274	1.425256104
O	5.025804364	-0.758670055	3.159791227

H	4.140683299	-1.031827075	2.927287212
H	5.552154399	-1.544063112	3.226183233
O	-0.264665017	-3.327435241	2.832781203
H	-0.002365999	-2.522987184	2.391665171
H	0.533658036	-3.727547270	3.149010225

Coord_2

C	-0.367493025	-0.277263018	0.202057014
N	0.333983024	-0.946383069	1.085242079
C	1.636560120	-0.617508045	1.282939090
C	1.376283099	1.037864072	-0.390286028
N	0.123079008	0.761646053	-0.563603039
N	2.152493158	0.417777029	0.521839037
H	3.107330224	0.701816051	0.669254049
N	-1.666373119	-0.562082041	0.024512003
H	-1.977725142	-1.456849102	0.356030024
H	-2.090216150	-0.228759017	-0.821380057
H	1.819912131	1.847309134	-0.951043067
O	2.345433167	-1.197668087	2.081917148
O	-2.748976196	0.409718030	-2.737848197
H	-2.620342187	-0.095803006	-3.528554256
H	-2.365659168	1.269630092	-2.883449205
O	-1.181122085	2.802998203	-2.340746170
H	-1.544216113	3.530386252	-1.852783134
H	-0.798047055	2.202807161	-1.707958122
O	4.878166351	1.228652087	1.180623087
H	5.162155370	2.092990150	1.444366102
H	5.146078373	0.618975046	1.867658132
O	-2.162849156	-3.864777277	0.722967054
H	-2.826355203	-4.527771329	0.863957060
H	-1.561509112	-3.911604283	1.461801106
O	5.040195360	-0.776793058	3.170882226
H	4.152326299	-1.051665073	2.953969212
H	5.567072403	-1.562092112	3.236787231
O	-0.278422022	-3.297652235	2.822904205
H	-0.021850004	-2.506912181	2.357866171
H	0.471070036	-3.661052265	3.276681237

Coord_3

C	-0.376743027	-0.236194016	0.176057011
N	0.327890024	-0.925842064	1.060981075
C	1.621022116	-0.593247040	1.260484088
C	1.391966098	1.047248073	-0.427806028
N	0.120413008	0.786980059	-0.585224041
N	2.152158157	0.439803032	0.514411039
H	3.109760222	0.710306049	0.667447047
N	-1.681990119	-0.513055039	0.021720001

H	-1.988758144	-1.410906103	0.348630026
H	-2.114098152	-0.178955014	-0.819790059
H	1.830882134	1.864222137	-0.980313072
O	2.329861169	-1.179691084	2.071830151
O	-2.764848201	0.454044033	-2.746350196
H	-2.611854189	-0.056326002	-3.529454254
H	-2.372415169	1.311285094	-2.884223206
O	-1.174778086	2.832674204	-2.349142170
H	-1.527167112	3.562504258	-1.857121134
H	-0.789231057	2.229123161	-1.720363121
O	4.889684354	1.210696087	1.181889085
H	5.182132372	2.074767148	1.437413105
H	5.157391373	0.603981041	1.871150136
O	-2.171551159	-4.042379290	0.762117052
H	-2.758101196	-4.772692345	0.916424064
H	-1.559417110	-4.021775287	1.491901110
O	5.055273366	-0.793067058	3.183171230
H	4.165456298	-1.071316076	2.981859213
H	5.584320401	-1.577189115	3.248297233
O	-0.287656022	-3.280410238	2.805370203
H	-0.036747005	-2.499169180	2.323938167
H	0.398132028	-3.595485261	3.381302241

Coord_4

C	-0.384910026	-0.201770014	0.151990009
N	0.323990025	-0.911311063	1.038074076
C	1.607096118	-0.572790043	1.239492087
C	1.406313104	1.051346075	-0.463379032
N	0.117096008	0.806454057	-0.604796043
N	2.151056156	0.458922032	0.508546036
H	3.110727225	0.717754049	0.666996050
N	-1.695750124	-0.472401033	0.021571000
H	-1.996753145	-1.373833098	0.343427023
H	-2.136932155	-0.137703012	-0.815097061
H	1.840649132	1.876083137	-1.006903070
O	2.316733165	-1.164367085	2.063231148
O	-2.781340201	0.490256035	-2.753246196
H	-2.604024186	-0.024596000	-3.528167253
H	-2.380517174	1.345046099	-2.882808208
O	-1.171629085	2.855469207	-2.354687170
H	-1.514128110	3.586956258	-1.858284133
H	-0.782980056	2.248621163	-1.730306124
O	4.898412355	1.195215086	1.184346087
H	5.197597376	2.059478148	1.431542105
H	5.167301370	0.591966045	1.875727133
O	-2.176871157	-4.181502301	0.797770057
H	-2.690438196	-4.964629357	0.957064067

H	-1.556008113	-4.110773296	1.515827108
O	5.071923368	-0.806598057	3.196476228
H	4.180919301	-1.089821076	3.010935217
H	5.604663403	-1.588512117	3.260664232
O	-0.291413021	-3.273211237	2.783810199
H	-0.046764002	-2.498466179	2.290601164
H	0.316965022	-3.531347254	3.466187251

Coord_5

C	-0.391937029	-0.173190014	0.129584009
N	0.322293022	-0.902105067	1.016221072
C	1.594798113	-0.555691040	1.219737086
C	1.419685100	1.050780077	-0.497188034
N	0.113424010	0.820842058	-0.622551046
N	2.149375155	0.475591036	0.504044034
H	3.110519226	0.724512050	0.667726050
N	-1.707621120	-0.439160029	0.023761000
H	-2.001823144	-1.344609094	0.340058026
H	-2.158606155	-0.103979006	-0.807589057
H	1.849665132	1.883522136	-1.030865073
O	2.305966165	-1.151381085	2.055910150
O	-2.798218203	0.519636035	-2.758834197
H	-2.596701188	0.000698001	-3.525022252
H	-2.389575170	1.372132100	-2.879469205
O	-1.171019086	2.872431206	-2.357572170
H	-1.504347110	3.604855260	-1.856447131
H	-0.778750056	2.262283165	-1.737990127
O	4.904822353	1.182382083	1.187863084
H	5.209121375	2.047293149	1.426638103
H	5.176171370	0.583063040	1.881254135
O	-2.181855155	-4.288882308	0.829937059
H	-2.628949192	-5.112985368	0.985593071
H	-1.552444110	-4.182898303	1.535205113
O	5.090315367	-0.817226058	3.210634233
H	4.198886303	-1.106913078	3.041004217
H	5.628156407	-1.595950116	3.273724237
O	-0.288459022	-3.274164237	2.760468201
H	-0.052113005	-2.504139181	2.257454163
H	0.230203015	-3.466813252	3.533311253

Coord_6

C	-0.398391028	-0.149012011	0.107202008
N	0.321797024	-0.897504067	0.993548071
C	1.583125113	-0.541777039	1.199990085
C	1.432169101	1.046847073	-0.529586038
N	0.109427008	0.831881061	-0.639395048
N	2.146634155	0.490277038	0.500436034

H	3.108726226	0.730693052	0.669600047
N	-1.718203126	-0.411485027	0.026089999
H	-2.004950142	-1.321446096	0.335680027
H	-2.179356158	-0.075339007	-0.799391059
H	1.858406135	1.888071134	-1.051805078
O	2.296103163	-1.141271080	2.048518147
O	-2.814931203	0.546069042	-2.765083198
H	-2.589292188	0.023834000	-3.522248252
H	-2.398723173	1.396353099	-2.875549208
O	-1.171740085	2.886712207	-2.357889169
H	-1.496551107	3.619176262	-1.851371136
H	-0.775721056	2.272790164	-1.743744125
O	4.908580353	1.171551084	1.193208086
H	5.216532375	2.037380146	1.424053104
H	5.183261372	0.576170041	1.888244138
O	-2.186354157	-4.377511316	0.864411063
H	-2.574000183	-5.233085378	1.010848071
H	-1.547006110	-4.246253308	1.555724114
O	5.108913365	-0.826743062	3.225333232
H	4.217829303	-1.124048080	3.071302223
H	5.653011407	-1.601453115	3.286891236
O	-0.276303021	-3.281116235	2.736715196
H	-0.054627004	-2.516092179	2.221508158
H	0.142617010	-3.393732244	3.583359260

Coord_7

C	-0.408003030	-0.123088009	0.077134003
N	0.316242023	-0.894926063	0.961294072
C	1.566014114	-0.531054040	1.174475084
C	1.442942102	1.044584073	-0.562216039
N	0.104087006	0.846948060	-0.659595046
N	2.139424152	0.503956037	0.495676038
H	3.102064223	0.735305054	0.672685049
N	-1.731542123	-0.381064030	0.018091004
H	-2.012086145	-1.296380092	0.316843020
H	-2.201420161	-0.040503004	-0.800754056
H	1.868152135	1.895538137	-1.068200079
O	2.278777165	-1.137560082	2.034731148
O	-2.829689205	0.587410041	-2.781495202
H	-2.579718186	0.064314007	-3.530411256
H	-2.404674174	1.435121106	-2.877559209
O	-1.168937086	2.912362212	-2.356169168
H	-1.485529107	3.643055264	-1.842054134
H	-0.770955053	2.291906163	-1.749200127
O	4.906320353	1.157511085	1.204370085
H	5.217456377	2.023461144	1.430632106
H	5.183193373	0.563755040	1.899506136

O	-2.176404159	-4.499754325	0.932577067
H	-2.502265179	-5.380185387	1.082032079
H	-1.524200110	-4.332104310	1.603423114
O	5.118091368	-0.846220060	3.239428233
H	4.227892302	-1.150562083	3.098451223
H	5.668299407	-1.617074115	3.297774237
O	-0.246753018	-3.286350237	2.713239195
H	-0.064966006	-2.534461181	2.168808158
H	0.069168007	-3.274005235	3.613083262

Coord_8

C	-0.383126027	-0.173025011	0.120639009
N	0.371931028	-0.934173066	1.009777074
C	1.605542115	-0.534045039	1.204202087
C	1.457227104	0.984359072	-0.573254041
N	0.105157008	0.778338055	-0.635207044
N	2.159374155	0.498963038	0.514453035
H	3.120358224	0.743843054	0.680495049
N	-1.705355125	-0.451919032	0.108610005
H	-1.958616139	-1.370474098	0.420916030
H	-2.201502157	-0.134507009	-0.704139049
H	1.859827134	1.840862131	-1.087223080
O	2.340979167	-1.113744079	2.080239148
O	-2.861796204	0.443381033	-2.706769193
H	-2.588606184	-0.092679008	-3.438278247
H	-2.444536175	1.293691093	-2.813321202
O	-1.220419089	2.791695199	-2.338787166
H	-1.535200112	3.526445252	-1.829468130
H	-0.801043056	2.185925158	-1.730685126
O	4.927731357	1.194471084	1.185397086
H	5.228086379	2.071330147	1.382494100
H	5.227687379	0.624215043	1.890156135
O	-2.272347164	-4.037391292	0.709162052
H	-2.678425195	-4.895670354	0.671276046
H	-1.626407119	-4.068261291	1.405998100
O	5.217579374	-0.761812056	3.265923233
H	4.333071313	-1.093000076	3.157647228
H	5.789343416	-1.516493109	3.330989238
O	-0.260003018	-3.369695241	2.677718193
H	0.033647000	-2.573793185	2.238968160
H	-0.139172008	-3.476904249	3.608675258

Coord_9

C	-0.383634027	-0.177627012	0.101790006
N	0.383744027	-0.956462070	0.986740073
C	1.602092117	-0.537677037	1.187044087
C	1.466488108	0.964669069	-0.596611041

N	0.100279009	0.767226058	-0.644562046
N	2.154687153	0.503668037	0.517255039
H	3.114238226	0.748801053	0.689601052
N	-1.706192125	-0.462776035	0.114800009
H	-1.945664140	-1.388680097	0.415529032
H	-2.215247160	-0.144395008	-0.689668051
H	1.862941136	1.834144130	-1.092189081
O	2.343158170	-1.117934083	2.074270150
O	-2.877469206	0.437958029	-2.709825197
H	-2.578259186	-0.096238005	-3.432580247
H	-2.457182178	1.288488090	-2.801429203
O	-1.234810091	2.782284200	-2.323310166
H	-1.546200109	3.512411254	-1.805430131
H	-0.808289058	2.172480156	-1.723569126
O	4.922560353	1.198532085	1.200100085
H	5.217855377	2.078331152	1.391808101
H	5.231233374	0.632997047	1.904507136
O	-2.285170165	-3.983255284	0.725415054
H	-2.704201197	-4.831201346	0.643748045
H	-1.629108119	-4.058977294	1.410164101
O	5.245907380	-0.759495053	3.283274235
H	4.366191315	-1.105728080	3.189493232
H	5.830780418	-1.504643111	3.344209239
O	-0.204812016	-3.414949246	2.653029191
H	0.056896005	-2.621112188	2.194218159
H	-0.221829018	-3.380905242	3.598780258

Coord_10

C	-0.373591026	-0.216509014	0.096070008
N	0.391908030	-1.007749071	0.993653070
C	1.592742116	-0.571826041	1.213374089
C	1.499077108	0.898384062	-0.590315044
N	0.118952008	0.714147050	-0.641966046
N	2.155088153	0.470830033	0.562369040
H	3.111154223	0.715774053	0.752050053
N	-1.697154121	-0.504147038	0.118751010
H	-1.929674139	-1.434006103	0.412078029
H	-2.207295161	-0.190024015	-0.686825052
H	1.899777138	1.775449129	-1.067684078
O	2.324976169	-1.146852085	2.127243153
O	-2.842168205	0.383047026	-2.740070196
H	-2.509548182	-0.156216013	-3.444381249
H	-2.414772172	1.231371090	-2.817512201
O	-1.196135087	2.720983196	-2.330915168
H	-1.509102106	3.451587251	-1.814755129
H	-0.772810058	2.110702152	-1.728699123
O	4.914020353	1.165513081	1.289280094

H	5.203465375	2.049216147	1.471849108
H	5.220375377	0.610337042	2.002503142
O	-2.284770166	-3.608108261	0.685903050
H	-2.832611205	-4.362884312	0.518890038
H	-1.676933121	-3.839280279	1.382490100
O	5.237757378	-0.776232056	3.396705247
H	4.363718317	-1.136281081	3.308363238
H	5.833102422	-1.512325108	3.468175248
O	-0.184234012	-3.475678252	2.664271191
H	0.055879006	-2.686603196	2.188077158
H	-0.394389030	-3.202874230	3.547525255

LIIC path connecting S2-MIN and S₁/T₁/S₀-III

Coord_1

C	-0.373591026	-0.216509014	0.096070008
N	0.391908030	-1.007749071	0.993653070
C	1.592742116	-0.571826041	1.213374089
C	1.499077108	0.898384062	-0.590315044
N	0.118952008	0.714147050	-0.641966046
N	2.155088153	0.470830033	0.562369040
H	3.111154223	0.715774053	0.752050053
N	-1.697154121	-0.504147038	0.118751010
H	-1.929674139	-1.434006103	0.412078029
H	-2.207295161	-0.190024015	-0.686825052
H	1.899777138	1.775449129	-1.067684078
O	2.324976169	-1.146852085	2.127243153
O	-2.842168205	0.383047026	-2.740070196
H	-2.509548182	-0.156216013	-3.444381249
H	-2.414772172	1.231371090	-2.817512201
O	-1.196135087	2.720983196	-2.330915168
H	-1.509102106	3.451587251	-1.814755129
H	-0.772810058	2.110702152	-1.728699123
O	4.914020353	1.165513081	1.289280094
H	5.203465375	2.049216147	1.471849108
H	5.220375377	0.610337042	2.002503142
O	-2.284770166	-3.608108261	0.685903050
H	-2.832611205	-4.362884312	0.518890038
H	-1.676933121	-3.839280279	1.382490100
O	5.237757378	-0.776232056	3.396705247
H	4.363718317	-1.136281081	3.308363238
H	5.833102422	-1.512325108	3.468175248
O	-0.184234012	-3.475678252	2.664271191
H	0.055879006	-2.686603196	2.188077158
H	-0.394389030	-3.202874230	3.547525255

Coord_2

C	-0.368060028	-0.222811017	0.079568007
---	--------------	--------------	-------------

N	0.408348028	-1.038021074	0.953040071
C	1.604017116	-0.576814039	1.217599088
C	1.514780110	0.866322065	-0.604043045
N	0.125185006	0.708580052	-0.653746050
N	2.155832155	0.475060033	0.572330040
H	3.109655223	0.727447052	0.762948056
N	-1.693960124	-0.491703033	0.125367012
H	-1.932505137	-1.425033103	0.400926031
H	-2.218597159	-0.155197014	-0.662474045
H	1.931644139	1.719798124	-1.109320077
O	2.307265168	-1.137349083	2.148796156
O	-2.856040205	0.383334025	-2.726894196
H	-2.524913183	-0.156151009	-3.431748248
H	-2.428735175	1.231596091	-2.805521204
O	-1.209218084	2.721137197	-2.323740165
H	-1.511542111	3.456226246	-1.807654131
H	-0.775114058	2.114499152	-1.725529124
O	4.918879354	1.172522087	1.293172092
H	5.203382374	2.055391148	1.487315107
H	5.216535376	0.611695043	2.005593146
O	-2.246766164	-3.592087261	0.690141051
H	-2.777513201	-4.357699312	0.517256039
H	-1.638420119	-3.813248277	1.389554102
O	5.201847373	-0.784146056	3.389979245
H	4.321256309	-1.126337079	3.294107240
H	5.782312418	-1.532106108	3.459605249
O	-0.159606013	-3.466296251	2.711962195
H	0.130400011	-2.695479192	2.266817161
H	-0.379513027	-3.202689229	3.594909257

Coord_3

C	-0.361884027	-0.229159017	0.061929005
N	0.426084033	-1.067657079	0.909403067
C	1.614309116	-0.582527042	1.221398088
C	1.530951110	0.832760061	-0.617163042
N	0.132311008	0.703214052	-0.666064047
N	2.155836155	0.478426034	0.582163042
H	3.107280222	0.738052055	0.774334056
N	-1.689151120	-0.481282035	0.133075007
H	-1.932377139	-1.418228101	0.390732029
H	-2.228310160	-0.122737011	-0.635637043
H	1.964713140	1.661206121	-1.149007085
O	2.286232166	-1.131194079	2.168750155
O	-2.868137208	0.384090029	-2.713668194
H	-2.538583180	-0.154800009	-3.419721245
H	-2.441446177	1.232601088	-2.792953202
O	-1.221652088	2.722327195	-2.315315166

H	-1.513055108	3.461440251	-1.798733129
H	-0.776027058	2.119145153	-1.722106125
O	4.922661352	1.180570084	1.296276092
H	5.201452374	2.062813150	1.501332107
H	5.212385377	0.614818046	2.008018143
O	-2.212798160	-3.576632258	0.694325049
H	-2.728805198	-4.351050311	0.516031036
H	-1.603541116	-3.790058275	1.395372099
O	5.167212373	-0.789098059	3.382982241
H	4.280678309	-1.113999079	3.280184237
H	5.733214411	-1.548140110	3.450689248
O	-0.134977008	-3.456914251	2.759652199
H	0.204921016	-2.704354193	2.345555169
H	-0.364637024	-3.202504229	3.642292264

Coord_4

C	-0.355349026	-0.235300018	0.043232003
N	0.444792031	-1.096309080	0.862726062
C	1.623224117	-0.589031043	1.224717088
C	1.547400114	0.797190058	-0.629994045
N	0.140193008	0.698047049	-0.679040050
N	2.154918155	0.480616034	0.591565040
H	3.103918222	0.747101055	0.785808058
N	-1.682981120	-0.472569031	0.142122012
H	-1.929731137	-1.413219100	0.381785028
H	-2.236758163	-0.092401005	-0.605994042
H	1.998951146	1.598915117	-1.187228087
O	2.261461162	-1.128558083	2.186937156
O	-2.878947209	0.386058029	-2.700245195
H	-2.551318185	-0.151574012	-3.408160246
H	-2.453110175	1.234977089	-2.779756198
O	-1.233070087	2.724760199	-2.305821165
H	-1.512956110	3.467575251	-1.788209127
H	-0.775332058	2.124752152	-1.718660123
O	4.925193354	1.189210083	1.298344096
H	5.197533372	2.071085149	1.513449107
H	5.207617374	0.619424047	2.009759147
O	-2.181215158	-3.561963259	0.698630049
H	-2.684285193	-4.343723312	0.515382037
H	-1.570279113	-3.769399269	1.400039099
O	5.133229367	-0.791066059	3.376130242
H	4.241312306	-1.099240082	3.266932236
H	5.685147410	-1.560460113	3.442180247
O	-0.110349009	-3.447531250	2.807342203
H	0.279442021	-2.713229194	2.424294177
H	-0.349760026	-3.202319229	3.689675266

Coord_5

C	-0.348743026	-0.241001020	0.023506000
N	0.464141032	-1.123654082	0.812947056
C	1.630355120	-0.596399042	1.227447087
C	1.563869110	0.759108055	-0.642828049
N	0.148683011	0.693098051	-0.692794049
N	2.152881156	0.481341033	0.600202043
H	3.099442224	0.754131053	0.796943059
N	-1.675649120	-0.465390033	0.152573009
H	-1.924902140	-1.409814103	0.374112027
H	-2.244118161	-0.064094007	-0.573460039
H	2.034207146	1.532147109	-1.224393089
O	2.232537159	-1.129598081	2.203094160
O	-2.888925206	0.390038029	-2.686507192
H	-2.563837186	-0.145789009	-3.396966242
H	-2.463915175	1.239386088	-2.765878197
O	-1.243131091	2.728720196	-2.295378164
H	-1.510598106	3.475009250	-1.776216129
H	-0.772835056	2.131483154	-1.715378123
O	4.926275352	1.197995087	1.299171094
H	5.191440372	2.079809149	1.523292111
H	5.201871377	0.625206044	2.010824142
O	-2.150259156	-3.548268257	0.703416050
H	-2.641567190	-4.336463312	0.515781037
H	-1.536615111	-3.750757270	1.403931102
O	5.099186368	-0.790090055	3.369799245
H	4.202405300	-1.082094077	3.254596236
H	5.637355407	-1.569158115	3.434790250
O	-0.085721005	-3.438149250	2.855032207
H	0.353963026	-2.722104195	2.503033180
H	-0.334884022	-3.202133228	3.737058268

Coord_6

C	-0.342377024	-0.246027018	0.002756003
N	0.483767036	-1.149358083	0.759983055
C	1.635256116	-0.604703045	1.229440090
C	1.580020113	0.718015050	-0.655928049
N	0.157614010	0.688427051	-0.707433050
N	2.149507153	0.480334035	0.607719043
H	3.093717224	0.758692053	0.807292057
N	-1.667345123	-0.459703034	0.164296010
H	-1.918156136	-1.407995099	0.367454025
H	-2.250438162	-0.037863003	-0.538237039
H	2.070204148	1.460096107	-1.260845093
O	2.199019157	-1.134444080	2.216896161
O	-2.898510209	0.396909030	-2.672357194
H	-2.576825185	-0.136658008	-3.386068244

H	-2.474041178	1.246571087	-2.751260199
O	-1.251505088	2.734571198	-2.284050162
H	-1.505357108	3.484170250	-1.762829125
H	-0.768352057	2.139562156	-1.712417123
O	4.925685357	1.206432088	1.298584094
H	5.182972372	2.088541150	1.530537108
H	5.194739375	0.631805043	2.011243145
O	-2.117981154	-3.535715252	0.709232052
H	-2.597945189	-4.330038312	0.518028035
H	-1.500444110	-3.733372268	1.407727102
O	5.064262363	-0.786284059	3.364335241
H	4.163109301	-1.062656074	3.243338234
H	5.588957401	-1.574408114	3.429190247
O	-0.061092005	-3.428766249	2.902722211
H	0.428484031	-2.730980196	2.581772188
H	-0.320008024	-3.201948233	3.784441270

Coord_7

C	-0.336616025	-0.250124019	-0.019054001
N	0.503224037	-1.173066087	0.703739049
C	1.637406115	-0.614009045	1.230512087
C	1.595396115	0.673418050	-0.669518051
N	0.166773009	0.684148050	-0.723054050
N	2.144527156	0.477339035	0.613744044
H	3.086565224	0.760319056	0.816379057
N	-1.658307119	-0.455588035	0.176901012
H	-1.909753140	-1.407903101	0.361171024
H	-2.255670164	-0.013891003	-0.500939039
H	2.106503151	1.381925097	-1.296855092
O	2.160386154	-1.143202085	2.227951161
O	-2.908129212	0.407663029	-2.657730190
H	-2.590946185	-0.123249011	-3.375434242
H	-2.483657180	1.257398091	-2.735842197
O	-1.257869090	2.742789199	-2.271845165
H	-1.496630108	3.495553249	-1.748056126
H	-0.761721053	2.149289153	-1.709891122
O	4.923171352	1.213935086	1.296434094
H	5.171903371	2.096735153	1.534903112
H	5.185737371	0.638748045	2.011061145
O	-2.082059152	-3.524427256	0.716896052
H	-2.550094183	-4.325304314	0.523384039
H	-1.459381104	-3.716069267	1.412523099
O	5.027480364	-0.779888057	3.360030242
H	4.122429298	-1.041120073	3.233221233
H	5.538886401	-1.576519113	3.425994244
O	-0.036464001	-3.419383249	2.950411215
H	0.503005037	-2.739855197	2.660511191

H -0.305132021 -3.201763233 3.831823277

Coord_8

C -0.331954026 -0.253017016 -0.042057002
N 0.521899035 -1.194423088 0.644041045
C 1.636119119 -0.624431043 1.230395091
C 1.609352117 0.624842044 -0.683794052
N 0.175858014 0.680455049 -0.739754053
N 2.137555156 0.472069033 0.617873045
H 3.077707221 0.758472053 0.823716057
N -1.648931120 -0.453257030 0.189583015
H -1.900068138 -1.409872101 0.354012023
H -2.259677163 0.007513999 -0.462851035
H 2.142437155 1.296796094 -1.332596093
O 2.115936154 -1.156020081 2.235751159
O -2.918213208 0.423503029 -2.642667191
H -2.606842188 -0.104365009 -3.365154244
H -2.492931181 1.272941090 -2.719609198
O -1.261919090 2.754023198 -2.258691163
H -1.483843106 3.509773253 -1.731792122
H -0.752825054 2.161098156 -1.707865124
O 4.918390352 1.219725089 1.292639094
H 5.157943373 2.103629153 1.536210111
H 5.174234370 0.645334047 2.010358143
O -2.039381145 -3.514402252 0.727738052
H -2.493416177 -4.323264309 0.534004039
H -1.410356102 -3.696829266 1.420150104
O 4.987602360 -0.771412056 3.357104241
H 4.079112293 -1.017903073 3.224173233
H 5.485767393 -1.576079113 3.425710245
O -0.011835002 -3.410001243 2.998101214
H 0.577526042 -2.748730198 2.739250199
H -0.290256023 -3.201577232 3.879206279

Coord_9

C -0.329166024 -0.254445016 -0.066715006
N 0.538829040 -1.213170086 0.580373042
C 1.630337117 -0.636293048 1.228559090
C 1.620905115 0.571869042 -0.698975051
N 0.184354013 0.677669047 -0.757721055
N 2.127904153 0.464095036 0.619634046
H 3.066571220 0.752385054 0.828813060
N -1.639982118 -0.453125033 0.200743014
H -1.889818138 -1.414537100 0.343536023
H -2.262208164 0.025940004 -0.426519032
H 2.176971156 1.203981087 -1.368119101
O 2.064531151 -1.173346085 2.239459163

O	-2.929225212	0.446074031	-2.627564187
H	-2.625132188	-0.078227008	-3.355735243
H	-2.502064182	1.294728095	-2.702720194
O	-1.263432092	2.769288199	-2.244357164
H	-1.466553107	3.527683252	-1.713664124
H	-0.741677052	2.175685155	-1.706310121
O	4.910708355	1.222624086	1.287317095
H	5.140534368	2.108019154	1.534619113
H	5.159217373	0.650357045	2.009335143
O	-1.984970145	-3.505206252	0.744335051
H	-2.420353172	-4.325119313	0.554189039
H	-1.348529096	-3.671608266	1.434026106
O	4.942830356	-0.762031056	3.355626243
H	4.031364291	-0.994025071	3.215858234
H	5.427607390	-1.574363113	3.428605247
O	0.012793003	-3.400618242	3.045791218
H	0.652047047	-2.757605199	2.817988202
H	-0.275380020	-3.201392232	3.926589281

Coord_10

C	-0.279066020	-0.221724018	-0.067443005
N	0.576741039	-1.195788084	0.576110043
C	1.644928116	-0.617284044	1.285418095
C	1.700646120	0.491885033	-0.685399051
N	0.267707018	0.679219050	-0.769785053
N	2.169191155	0.458764035	0.655589047
H	3.109632225	0.735103051	0.871959062
N	-1.589551114	-0.390287028	0.223329018
H	-1.856962132	-1.348902098	0.364873026
H	-2.202189156	0.101146008	-0.402471027
H	2.300010164	1.050128078	-1.382207101
O	2.008146145	-1.141668085	2.318607167
O	-2.846417207	0.488158038	-2.638677189
H	-2.552359183	-0.057574003	-3.355138241
H	-2.399043172	1.324826094	-2.729082196
O	-1.127765080	2.778486199	-2.297183166
H	-1.301762094	3.556863255	-1.785377129
H	-0.611774044	2.187477155	-1.750850129
O	4.959872355	1.192614085	1.331232097
H	5.193482372	2.082156151	1.559083115
H	5.180235372	0.639821047	2.077220149
O	-1.929670138	-3.406028244	0.871079061
H	-2.349978170	-4.240188307	0.711322053
H	-1.295928095	-3.534091255	1.571384115
O	4.888650352	-0.722688050	3.459663247
H	3.972543287	-0.927002068	3.306458237
H	5.342839386	-1.548621111	3.567457256

O	0.039307000	-3.393977243	3.092942223
H	0.728402053	-2.769150200	2.896238208
H	-0.258807019	-3.203881233	3.973354288

LIIC path connecting S₁/T₁/S₀-III and S₀-MIN

Coord_1

C	-0.279066020	-0.221724018	-0.067443005
N	0.576741039	-1.195788084	0.576110043
C	1.644928116	-0.617284044	1.285418095
C	1.700646120	0.491885033	-0.685399051
N	0.267707018	0.679219050	-0.769785053
N	2.169191155	0.458764035	0.655589047
H	3.109632225	0.735103051	0.871959062
N	-1.589551114	-0.390287028	0.223329018
H	-1.856962132	-1.348902098	0.364873026
H	-2.202189156	0.101146008	-0.402471027
H	2.300010164	1.050128078	-1.382207101
O	2.008146145	-1.141668085	2.318607167
O	-2.846417207	0.488158038	-2.638677189
H	-2.552359183	-0.057574003	-3.355138241
H	-2.399043172	1.324826094	-2.729082196
O	-1.127765080	2.778486199	-2.297183166
H	-1.301762094	3.556863255	-1.785377129
H	-0.611774044	2.187477155	-1.750850129
O	4.959872355	1.192614085	1.331232097
H	5.193482372	2.082156151	1.559083115
H	5.180235372	0.639821047	2.077220149
O	-1.929670138	-3.406028244	0.871079061
H	-2.349978170	-4.240188307	0.711322053
H	-1.295928095	-3.534091255	1.571384115
O	4.888650352	-0.722688050	3.459663247
H	3.972543287	-0.927002068	3.306458237
H	5.342839386	-1.548621111	3.567457256
O	0.039307000	-3.393977243	3.092942223
H	0.728402053	-2.769150200	2.896238208
H	-0.258807019	-3.203881233	3.973354288

Coord_2

C	-0.286653019	-0.233602016	-0.044906003
N	0.551740039	-1.181877084	0.636250048
C	1.659742121	-0.621718046	1.282280095
C	1.678558119	0.578130039	-0.662585045
N	0.254175020	0.684691049	-0.753220053
N	2.188556158	0.452629035	0.647157047
H	3.130468224	0.728270050	0.858604062
N	-1.601105117	-0.400440029	0.200290017
H	-1.872878132	-1.351434100	0.374350024

H	-2.205319160	0.075358005	-0.446481032
H	2.257576165	1.174865083	-1.345446099
O	2.076830151	-1.141620083	2.295906166
O	-2.825548202	0.463804036	-2.667541194
H	-2.544363182	-0.079736005	-3.390629244
H	-2.387550172	1.304402096	-2.766967201
O	-1.130734082	2.771945198	-2.321363169
H	-1.332250096	3.548046257	-1.816215129
H	-0.631775044	2.184879160	-1.755679125
O	4.973795358	1.181709086	1.327786094
H	5.218595378	2.066160149	1.563517112
H	5.192904373	0.618661042	2.066759151
O	-1.951019138	-3.411805245	0.885642061
H	-2.418353173	-4.224713307	0.748915054
H	-1.325133096	-3.556694257	1.590102114
O	4.906424353	-0.748035053	3.437055250
H	3.991792289	-0.952285067	3.272552236
H	5.361215388	-1.574070113	3.540329254
O	0.039074004	-3.394261247	3.092885220
H	0.728403053	-2.769020197	2.896463208
H	-0.258575017	-3.203730232	3.973189285

Coord_3

C	-0.292512022	-0.245048019	-0.017960001
N	0.527961036	-1.164596086	0.699461048
C	1.671751121	-0.625532044	1.283792092
C	1.654077120	0.655475046	-0.632092048
N	0.243672015	0.690205050	-0.732085053
N	2.204320158	0.445686033	0.639693044
H	3.147807225	0.721181054	0.845269060
N	-1.610564118	-0.413973028	0.176042015
H	-1.887254137	-1.356930098	0.379304028
H	-2.201263159	0.045270002	-0.495366035
H	2.214203157	1.286488091	-1.300656092
O	2.138494154	-1.143481083	2.275207165
O	-2.801159201	0.443864034	-2.691574192
H	-2.534596184	-0.097527007	-3.421648244
H	-2.371254170	1.287564094	-2.799574204
O	-1.127380082	2.767238198	-2.339924167
H	-1.354992097	3.540394253	-1.841374131
H	-0.646428047	2.182800155	-1.756649128
O	4.983835359	1.173736083	1.322614096
H	5.238764376	2.053760150	1.564018110
H	5.202778376	0.602382042	2.055588151
O	-1.973435140	-3.420908248	0.893692064
H	-2.485851181	-4.210182301	0.782674054
H	-1.356937099	-3.578224256	1.604085115

O	4.924088353	-0.766024053	3.416689244
H	4.011239289	-0.971731072	3.241816235
H	5.380732387	-1.591282116	3.516877251
O	0.038841002	-3.394544245	3.092828222
H	0.728404053	-2.768890200	2.896688209
H	-0.258343021	-3.203577231	3.973022288

Coord_4

C	-0.296714023	-0.255564020	0.012906003
N	0.505059038	-1.143531085	0.764979054
C	1.681112118	-0.628593043	1.289525092
C	1.628110117	0.724558051	-0.595549041
N	0.235875017	0.695975050	-0.707373052
N	2.216749161	0.438051032	0.632998047
H	3.161894230	0.713831052	0.831956061
N	-1.617311117	-0.430235031	0.151624009
H	-1.899832135	-1.364773097	0.381315029
H	-2.189979158	0.011533000	-0.546905041
H	2.171022156	1.385883099	-1.249796089
O	2.192905159	-1.147140084	2.256754162
O	-2.773993199	0.427569031	-2.711004194
H	-2.523867179	-0.111798007	-3.448272247
H	-2.351055167	1.273637091	-2.827438201
O	-1.118657082	2.764024198	-2.354083167
H	-1.370921099	3.533798255	-1.862190133
H	-0.656385046	2.181154159	-1.754886126
O	4.990105358	1.168678085	1.316309097
H	5.253986377	2.044935146	1.561650111
H	5.209905378	0.590615045	2.044134146
O	-1.996886143	-3.432986247	0.895616063
H	-2.552408185	-4.196074303	0.812572060
H	-1.390460102	-3.598542260	1.613079118
O	4.941549355	-0.777709054	3.398298245
H	4.030839289	-0.986456069	3.213704234
H	5.401355388	-1.601316116	3.496536249
O	0.038608005	-3.394827244	3.092770225
H	0.728404053	-2.768759202	2.896912210
H	-0.258111019	-3.203425230	3.972855285

Coord_5

C	-0.299276024	-0.264769021	0.047283003
N	0.482798033	-1.118333083	0.832106062
C	1.688023120	-0.630780043	1.299067095
C	1.601410114	0.786113055	-0.554380040
N	0.230548017	0.702143050	-0.679933047
N	2.226090161	0.429821030	0.626885044
H	3.172947230	0.706219049	0.818665060

N	-1.620863119	-0.448631032	0.128008008
H	-1.910335139	-1.374386099	0.381804026
H	-2.171450155	-0.025229002	-0.599098042
H	2.128937155	1.474072107	-1.194548085
O	2.239973163	-1.152476086	2.240813163
O	-2.744694200	0.414199029	-2.726086195
H	-2.512884179	-0.123291007	-3.470637251
H	-2.327754170	1.261986089	-2.851031204
O	-1.105410082	2.761946198	-2.364835170
H	-1.380867097	3.528067254	-1.879698137
H	-0.662199048	2.179803159	-1.751319128
O	4.992681361	1.166486085	1.309425094
H	5.264235381	2.039611146	1.557397114
H	5.214292373	0.583000042	2.032781146
O	-2.021326146	-3.447683246	0.891679064
H	-2.617842190	-4.181945302	0.838633061
H	-1.424887103	-3.617428263	1.616766118
O	4.958637356	-0.784032055	3.381620245
H	4.050482290	-0.997427072	3.187690229
H	5.422949392	-1.605114116	3.478779251
O	0.038375003	-3.395110243	3.092713222
H	0.728405054	-2.768629199	2.897137211
H	-0.257878017	-3.203273229	3.972688287

Coord_6

C	-0.300153024	-0.272374018	0.084870008
N	0.461077032	-1.088721080	0.900239067
C	1.692741122	-0.631964045	1.312040092
C	1.574595115	0.840921059	-0.509795037
N	0.227530019	0.708779049	-0.650461044
N	2.232588161	0.421088028	0.621178042
H	3.181183228	0.698365053	0.805395057
N	-1.620856118	-0.468622036	0.106108008
H	-1.918488136	-1.385230100	0.382086030
H	-2.145735157	-0.064444004	-0.650150047
H	2.088640149	1.552142114	-1.136335084
O	2.279783162	-1.159281083	2.227667162
O	-2.713837197	0.403091027	-2.737125198
H	-2.502293178	-0.132628011	-3.488955251
H	-2.302080167	1.252021089	-2.870790206
O	-1.088394081	2.760630198	-2.372986172
H	-1.385567101	3.522936251	-1.894651135
H	-0.664328049	2.178546157	-1.746718127
O	4.991635357	1.167087082	1.302457094
H	5.269495382	2.037685148	1.552149109
H	5.215925377	0.579199041	2.021866145
O	-2.046737148	-3.464640249	0.881989061

H	-2.681876193	-4.167449301	0.860845064
H	-1.459503106	-3.634558260	1.614747116
O	4.975138357	-0.785813059	3.366413241
H	4.070023293	-1.005455072	3.163286226
H	5.445315391	-1.603490114	3.463136248
O	0.038142001	-3.395393247	3.092656224
H	0.728405054	-2.768498201	2.897361206
H	-0.257645020	-3.203120228	3.972520284

Coord_7

C	-0.299247020	-0.278178018	0.125528009
N	0.439937031	-1.054488075	0.968964067
C	1.695593123	-0.631957044	1.328127096
C	1.548147111	0.889780063	-0.462791032
N	0.226725019	0.715887054	-0.619488046
N	2.236491161	0.411967028	0.615728046
H	3.186814229	0.690313050	0.792140056
N	-1.617000115	-0.489718036	0.086782005
H	-1.924003137	-1.396790099	0.383406025
H	-2.112932152	-0.105615005	-0.698476048
H	2.050616149	1.621185118	-1.076339079
O	2.312648165	-1.167165083	2.217627161
O	-2.681975191	0.393632026	-2.744514200
H	-2.492739179	-0.140295012	-3.503575254
H	-2.274733166	1.243205091	-2.887142206
O	-1.068303078	2.759664201	-2.379163173
H	-1.385674101	3.518050252	-1.907525140
H	-0.663142047	2.177093158	-1.741716127
O	4.987037357	1.170413083	1.295821095
H	5.269771380	2.039051145	1.546670114
H	5.214787376	0.578922043	2.011661147
O	-2.073141150	-3.483458253	0.866468065
H	-2.744145200	-4.152340301	0.879066066
H	-1.493711108	-3.649442264	1.606515118
O	4.990823361	-0.783725058	3.352456239
H	4.089307295	-1.011167075	3.140050227
H	5.468207392	-1.597105114	3.449195248
O	0.037909004	-3.395676246	3.092599221
H	0.728405054	-2.768368198	2.897586207
H	-0.257412018	-3.202968233	3.972352286

Coord_8

C	-0.296417022	-0.282057019	0.169380012
N	0.419584032	-1.015492072	1.038213075
C	1.696995120	-0.630435046	1.347129095
C	1.522418111	0.933471070	-0.414138031
N	0.228072018	0.723380050	-0.587332040

N	2.238034162	0.402643031	0.610426044
H	3.190045232	0.682164048	0.778894056
N	-1.608998118	-0.511446038	0.070840006
H	-1.926524137	-1.408532103	0.386976030
H	-2.073081147	-0.148310010	-0.742707053
H	2.015132142	1.682238123	-1.015537073
O	2.339213170	-1.175391085	2.211052161
O	-2.649706190	0.385248028	-2.748803198
H	-2.484963179	-0.146617013	-3.515072254
H	-2.246453161	1.235044088	-2.900542207
O	-1.045821078	2.758564200	-2.383820171
H	-1.381771101	3.512922254	-1.918474140
H	-0.658923049	2.175013158	-1.736843124
O	4.978958361	1.176434083	1.289808091
H	5.265100380	2.043640149	1.541543111
H	5.210869374	0.581969040	2.002338145
O	-2.100563153	-3.503622250	0.844782063
H	-2.804153201	-4.136463295	0.892854065
H	-1.527029108	-3.661326262	1.591401112
O	5.005469363	-0.778236056	3.339534238
H	4.108184296	-1.014957074	3.117586224
H	5.491361395	-1.586418115	3.436599247
O	0.037676002	-3.395959244	3.092542223
H	0.728405054	-2.768238200	2.897811208
H	-0.257179021	-3.202815232	3.972184288

Coord_9

C	-0.291481021	-0.283963021	0.216994015
N	0.400406030	-0.971635068	1.108549082
C	1.697473120	-0.626792047	1.369077097
C	1.497601106	0.972739070	-0.364370027
N	0.231510019	0.731048051	-0.554018041
N	2.237414162	0.393434029	0.605237043
H	3.191035228	0.674113050	0.765640055
N	-1.596404113	-0.533277039	0.059072003
H	-1.925521140	-1.419806102	0.394044028
H	-2.025941143	-0.192112016	-0.781673057
H	1.982201141	1.736226125	-0.954773068
O	2.360619168	-1.182615085	2.208391161
O	-2.617795188	0.377372029	-2.750822199
H	-2.479995178	-0.151682012	-3.524430256
H	-2.218159159	1.227092088	-2.911528207
O	-1.021695072	2.756694199	-2.387221172
H	-1.374354100	3.506848252	-1.927203141
H	-0.651832047	2.171626159	-1.732581125
O	4.967453359	1.185231083	1.284512090
H	5.255532379	2.051499145	1.537074109

H	5.204161375	0.588324041	1.993901144
O	-2.128917152	-3.524382254	0.816211059
H	-2.861176204	-4.119726297	0.901192067
H	-1.559040114	-3.669050265	1.568456114
O	5.018882360	-0.769497053	3.327411237
H	4.126525299	-1.016874071	3.095538224
H	5.514513397	-1.571567115	3.425023246
O	0.037443005	-3.396241243	3.092485220
H	0.728405054	-2.768108197	2.898037209
H	-0.256946019	-3.202662231	3.972016285

Coord_10

C	-0.357476028	-0.325875023	0.229680018
N	0.341885027	-0.973917071	1.110492078
C	1.653274120	-0.646333049	1.306678092
C	1.358668096	1.022653073	-0.350634025
N	0.124605007	0.729787053	-0.539943037
N	2.151526155	0.392262029	0.530966037
H	3.102758223	0.691790052	0.672735046
N	-1.649147119	-0.620508046	0.029419001
H	-1.963775141	-1.512845109	0.364878027
H	-2.065503149	-0.287993023	-0.820383060
H	1.807123128	1.824952131	-0.918745067
O	2.363013171	-1.219113085	2.093251151
O	-2.733839197	0.356619025	-2.728166195
H	-2.629401188	-0.143525009	-3.525973252
H	-2.360519169	1.219526087	-2.880668210
O	-1.191319087	2.765921198	-2.329191167
H	-1.566105111	3.489871251	-1.844840131
H	-0.810044059	2.169065158	-1.692877120
O	4.862872351	1.248671090	1.181207087
H	5.136525369	2.113660152	1.453307107
H	5.132414370	0.636409044	1.865785136
O	-2.145668152	-3.642177264	0.683196049
H	-2.886480206	-4.220391304	0.804450057
H	-1.559679111	-3.776041274	1.425256104
O	5.025804364	-0.758670055	3.159791227
H	4.140683299	-1.031827075	2.927287212
H	5.552154399	-1.544063112	3.226183233
O	-0.264665017	-3.327435241	2.832781203
H	-0.002365999	-2.522987184	2.391665171
H	0.533658036	-3.727547270	3.149010225

Relaxation pathway III

LIIC path connecting S1-MIN and S₁/T₁

Coord_1

C	-0.528514036	-0.198852015	0.053044002
---	--------------	--------------	-------------

N	0.272746019	-0.910152065	0.884654066
C	1.562816111	-0.642046047	1.248051090
C	1.456630102	0.873824062	-0.582809040
N	0.070876006	0.748146053	-0.594151045
N	2.110098154	0.394877027	0.566599039
H	3.079049219	0.607218045	0.725546052
N	-1.853804134	-0.459780034	0.017630000
H	-2.085728150	-1.385158100	0.332370023
H	-2.292495164	-0.199327015	-0.848195061
H	1.847113132	1.792133130	-0.988200073
O	2.132379151	-1.281374091	2.107923151
O	-2.789862203	0.433758029	-2.797952202
H	-2.500767179	-0.039636000	-3.565975258
H	-2.439824174	1.317267093	-2.865880208
O	-1.341935098	2.902234209	-2.304437165
H	-1.692337122	3.660765265	-1.855336134
H	-0.901531063	2.370124170	-1.651441118
O	4.913998355	1.132336081	1.249375092
H	5.124980367	2.000144144	1.565857113
H	5.128620371	0.515414037	1.946282139
O	-1.803395127	-3.468521251	0.881142065
H	-2.442738174	-4.155033300	1.014047074
H	-1.175779083	-3.528008256	1.597332115
O	4.875443353	-0.958641068	3.189077229
H	3.977989288	-1.155925083	2.933095212
H	5.358459386	-1.774142130	3.157625225
O	0.244686019	-3.374689245	3.029956218
H	0.891092063	-2.702802195	2.833502202
H	0.717654050	-4.099522294	3.415423246

Coord_2

C	-0.529093036	-0.199794014	0.054078004
N	0.271601022	-0.909292067	0.886833065
C	1.561858115	-0.641036048	1.248804088
C	1.456410107	0.872311065	-0.583106041
N	0.070081007	0.748952054	-0.591510043
N	2.108810152	0.397500026	0.568403042
H	3.078572219	0.607632041	0.725400052
N	-1.854223131	-0.460793033	0.017414001
H	-2.086601149	-1.385627099	0.333441025
H	-2.292230163	-0.201196016	-0.848993060
H	1.848012136	1.787995128	-0.993335072
O	2.132698155	-1.280538091	2.107663150
O	-2.787034201	0.433387033	-2.798718201
H	-2.498287179	-0.039263005	-3.567346256
H	-2.437559174	1.317145097	-2.866207208
O	-1.342603094	2.904379208	-2.303834168

H	-1.694903123	3.663960263	-1.857969135
H	-0.902857065	2.375043169	-1.648186117
O	4.914530353	1.131518084	1.248808089
H	5.124742369	1.999309145	1.565847111
H	5.128787368	0.514482039	1.945728138
O	-1.803927130	-3.469379248	0.881876066
H	-2.441591177	-4.157555300	1.014337074
H	-1.175598083	-3.528460253	1.597485116
O	4.875328352	-0.959327067	3.188790230
H	3.977802287	-1.156105083	2.932665214
H	5.358006384	-1.775011129	3.156914228
O	0.245394016	-3.374916241	3.029182217
H	0.891171064	-2.702472195	2.832499205
H	0.718630049	-4.098221296	3.417196244

Coord_3

C	-0.529671040	-0.200745014	0.055111006
N	0.270454020	-0.908442065	0.889008063
C	1.560898113	-0.640038046	1.249557091
C	1.456187107	0.870759062	-0.583395041
N	0.069294004	0.749742052	-0.588862045
N	2.107518150	0.400110029	0.570207039
H	3.078082222	0.608027046	0.725250051
N	-1.854639133	-0.461812033	0.017196001
H	-2.087473149	-1.386098099	0.334508026
H	-2.291958165	-0.203069012	-0.849793060
H	1.848905133	1.783786126	-0.998458074
O	2.133009153	-1.279715093	2.107402149
O	-2.784195202	0.433028029	-2.799475200
H	-2.495797178	-0.038871001	-3.568710258
H	-2.435281177	1.317034096	-2.866518206
O	-1.343252099	2.906515211	-2.303196165
H	-1.697432125	3.667133263	-1.860567136
H	-0.904186067	2.379945170	-1.644910119
O	4.915045354	1.130713084	1.248216088
H	5.124478368	1.998493143	1.565797114
H	5.128949371	0.513576035	1.945155140
O	-1.804466129	-3.470224249	0.882590063
H	-2.440456176	-4.160051297	1.014600075
H	-1.175431085	-3.528901254	1.597623115
O	4.875237350	-0.959971070	3.188507231
H	3.977639285	-1.156257083	2.932248211
H	5.357586386	-1.775833126	3.156216227
O	0.246078020	-3.375142242	3.028401220
H	0.891233062	-2.702149196	2.831489201
H	0.719569053	-4.096915297	3.418960246

Coord_4

C	-0.530246039	-0.201705016	0.056144002
N	0.269306017	-0.907604066	0.891180065
C	1.559937111	-0.639051046	1.250310090
C	1.455962106	0.869168065	-0.583675044
N	0.068515007	0.750516053	-0.586210041
N	2.106222153	0.402707030	0.572011041
H	3.077580223	0.608405042	0.725098050
N	-1.855053135	-0.462835033	0.016976001
H	-2.088345148	-1.386572099	0.335572027
H	-2.291679167	-0.204948015	-0.850596060
H	1.849793135	1.779506130	-1.003568074
O	2.133312154	-1.278907093	2.107140154
O	-2.781347202	0.432683032	-2.800226203
H	-2.493297181	-0.038459004	-3.570068259
H	-2.432990173	1.316936093	-2.866812206
O	-1.343881095	2.908643207	-2.302523168
H	-1.699926121	3.670286265	-1.863129132
H	-0.905520065	2.384831170	-1.641614117
O	4.915545352	1.129921080	1.247598088
H	5.124189368	1.997697144	1.565706112
H	5.129109367	0.512696039	1.944564139
O	-1.805011129	-3.471058248	0.883283063
H	-2.439334177	-4.162521301	1.014839073
H	-1.175279085	-3.529333253	1.597746117
O	4.875171351	-0.960574068	3.188229228
H	3.977502286	-1.156383086	2.931847211
H	5.357201383	-1.776608127	3.155531228
O	0.246738015	-3.375369243	3.027614217
H	0.891279064	-2.701835192	2.830473202
H	0.720474052	-4.095606293	3.420719247

Coord_5

C	-0.530820037	-0.202673013	0.057175003
N	0.268156020	-0.906776067	0.893348062
C	1.558974115	-0.638075048	1.251062087
C	1.455734105	0.867538061	-0.583947041
N	0.067744007	0.751273052	-0.583552042
N	2.104921149	0.405291029	0.573814043
H	3.077065223	0.608765042	0.724943054
N	-1.855464131	-0.463864034	0.016755001
H	-2.089217148	-1.387047099	0.336633022
H	-2.291394163	-0.206831013	-0.851402060
H	1.850675136	1.775155128	-1.008666072
O	2.133607155	-1.278112094	2.106877153
O	-2.778488200	0.432350031	-2.800970200
H	-2.490786182	-0.038028005	-3.571422260

H	-2.430686172	1.316850096	-2.867092204
O	-1.344491098	2.910764208	-2.301815166
H	-1.702382123	3.673419264	-1.865655133
H	-0.906857063	2.389700172	-1.638298118
O	4.916028353	1.129141083	1.246954090
H	5.123875371	1.996920142	1.565575114
H	5.129266369	0.511843037	1.943955141
O	-1.805564130	-3.471879251	0.883958066
H	-2.438225175	-4.164967301	1.015052072
H	-1.175141086	-3.529756256	1.597854117
O	4.875129350	-0.961136070	3.187956231
H	3.977391286	-1.156483084	2.931460214
H	5.356850385	-1.777336127	3.154860226
O	0.247375018	-3.375597245	3.026822219
H	0.891307063	-2.701528196	2.829451202
H	0.721343051	-4.094293293	3.422471247

Coord_6

C	-0.531393036	-0.203650017	0.058205005
N	0.267004017	-0.905960065	0.895513064
C	1.558008112	-0.637111045	1.251815091
C	1.455503103	0.865869062	-0.584211043
N	0.066980007	0.752014053	-0.580888042
N	2.103616151	0.407862031	0.575617040
H	3.076538220	0.609107044	0.724785053
N	-1.855873133	-0.464898036	0.016530000
H	-2.090089153	-1.387525099	0.337688027
H	-2.291102163	-0.208719017	-0.852211061
H	1.851552136	1.770733128	-1.013751074
O	2.133894154	-1.277331092	2.106614152
O	-2.775620202	0.432031033	-2.801707201
H	-2.488264181	-0.037578004	-3.572771259
H	-2.428368175	1.316777096	-2.867355205
O	-1.345082099	2.912877207	-2.301072164
H	-1.704802124	3.676533266	-1.868145134
H	-0.908198067	2.394552172	-1.634960115
O	4.916496352	1.128375083	1.246285088
H	5.123536369	1.996162144	1.565403110
H	5.129420370	0.511015039	1.943327140
O	-1.806123131	-3.472689252	0.884613066
H	-2.437130175	-4.167389297	1.015242073
H	-1.175016084	-3.530169252	1.597948114
O	4.875112353	-0.961658072	3.187689229
H	3.977305284	-1.156557085	2.931087212
H	5.356534387	-1.778017125	3.154202226
O	0.247990017	-3.375824240	3.026025220
H	0.891320064	-2.701230195	2.828424201

H	0.722179050	-4.092976292	3.424218246
---	-------------	--------------	-------------

Coord_7

C	-0.531964039	-0.204635017	0.059234006
N	0.265849019	-0.905154065	0.897674065
C	1.557041110	-0.636158045	1.252568089
C	1.455268106	0.864160063	-0.584465042
N	0.066224003	0.752739052	-0.578219042
N	2.102306151	0.410420032	0.577419042
H	3.075997221	0.609432043	0.724625051
N	-1.856280133	-0.465937033	0.016303004
H	-2.090963152	-1.388006100	0.338740026
H	-2.290804167	-0.210612016	-0.853023062
H	1.852423135	1.766239127	-1.018823074
O	2.134173152	-1.276563091	2.106349150
O	-2.772741197	0.431725030	-2.802439201
H	-2.485731179	-0.037107004	-3.574115258
H	-2.426037176	1.316717093	-2.867604204
O	-1.345652097	2.914983211	-2.300294168
H	-1.707185121	3.679627264	-1.870598135
H	-0.909542066	2.399388174	-1.631602115
O	4.916947354	1.127621080	1.245589088
H	5.123172369	1.995424142	1.565191111
H	5.129571371	0.510213039	1.942681141
O	-1.806688129	-3.473489252	0.885249063
H	-2.436046177	-4.169787301	1.015407076
H	-1.174906083	-3.530574253	1.598029115
O	4.875121349	-0.962138067	3.187425228
H	3.977245286	-1.156604081	2.930728213
H	5.356251383	-1.778652128	3.153557228
O	0.248582018	-3.376053242	3.025223220
H	0.891316064	-2.700939195	2.827392205
H	0.722980050	-4.091654296	3.425959244

Coord_8

C	-0.532534037	-0.205629013	0.060262007
N	0.264692020	-0.904359066	0.899831066
C	1.556070112	-0.635217046	1.253320092
C	1.455030103	0.862412064	-0.584711041
N	0.065474006	0.753448055	-0.575545040
N	2.100992151	0.412966030	0.579221044
H	3.075444221	0.609739045	0.724461053
N	-1.856685134	-0.466982036	0.016072002
H	-2.091837152	-1.388489102	0.339786024
H	-2.290500166	-0.212510016	-0.853840059
H	1.853288133	1.761673126	-1.023883072
O	2.134444155	-1.275808093	2.106084154

O	-2.769851202	0.431433030	-2.803164201
H	-2.483187181	-0.036615002	-3.575456257
H	-2.423691174	1.316669096	-2.867837206
O	-1.346202098	2.917082208	-2.299480166
H	-1.709530122	3.682703266	-1.873013136
H	-0.910890066	2.404206175	-1.628222117
O	4.917382354	1.126880084	1.244867089
H	5.122782371	1.994705144	1.564938112
H	5.129718371	0.509437038	1.942016140
O	-1.807260132	-3.474277250	0.885866062
H	-2.434976175	-4.172162302	1.015550075
H	-1.174809085	-3.530969252	1.598095114
O	4.875153353	-0.962577067	3.187166227
H	3.977210286	-1.156625084	2.930384211
H	5.356003384	-1.779240128	3.152925226
O	0.249151016	-3.376281243	3.024416219
H	0.891296066	-2.700656196	2.826355203
H	0.723747050	-4.090329295	3.427695247

Coord_9

C	-0.533104041	-0.206633016	0.061288002
N	0.263532022	-0.903576064	0.901986066
C	1.555097113	-0.634286043	1.254072090
C	1.454789105	0.860624064	-0.584948044
N	0.064732004	0.754140054	-0.572865043
N	2.099671150	0.415499033	0.581023041
H	3.074877223	0.610028045	0.724294050
N	-1.857089134	-0.468031035	0.015839000
H	-2.092712152	-1.388974098	0.340828027
H	-2.290190163	-0.214413017	-0.854661062
H	1.854146136	1.757036126	-1.028929073
O	2.134707156	-1.275065091	2.105818152
O	-2.766950199	0.431155032	-2.803885199
H	-2.480630180	-0.036103001	-3.576793255
H	-2.421330176	1.316635097	-2.868055206
O	-1.346731095	2.919174210	-2.298630165
H	-1.711837123	3.685759265	-1.875391137
H	-0.912239066	2.409008172	-1.624820116
O	4.917800356	1.126152079	1.244118091
H	5.122368369	1.994004143	1.564643111
H	5.129862371	0.508687035	1.941332141
O	-1.807838131	-3.475055251	0.886465064
H	-2.433918175	-4.174514299	1.015669071
H	-1.174725084	-3.531357255	1.598148117
O	4.875211351	-0.962975067	3.186912228
H	3.977200285	-1.156620083	2.930054211
H	5.355789385	-1.779783127	3.152304226

O	0.249698016	-3.376510245	3.023606218
H	0.891260066	-2.700380193	2.825312205
H	0.724481051	-4.088999292	3.429427245

Coord_10

C	-0.533673038	-0.207645014	0.062313002
N	0.262369017	-0.902803063	0.904136065
C	1.554121109	-0.633366047	1.254824088
C	1.454543107	0.858796063	-0.585176040
N	0.063997003	0.754815052	-0.570179040
N	2.098345148	0.418020028	0.582824043
H	3.074295223	0.610300042	0.724124052
N	-1.857491134	-0.469087034	0.015601003
H	-2.093587152	-1.389462100	0.341863023
H	-2.289872165	-0.216321018	-0.855486060
H	1.854996132	1.752325125	-1.033960072
O	2.134961155	-1.274335091	2.105551151
O	-2.764036200	0.430891031	-2.804599202
H	-2.478059178	-0.035569003	-3.578125258
H	-2.418954175	1.316614094	-2.868257209
O	-1.347239095	2.921258211	-2.297742168
H	-1.714106124	3.688796266	-1.877729137
H	-0.913591066	2.413792173	-1.621395117
O	4.918200356	1.125437081	1.243343090
H	5.121926368	1.993323145	1.564308110
H	5.130001370	0.507962036	1.940628140
O	-1.808420131	-3.475823251	0.887045064
H	-2.432870177	-4.176843303	1.015764075
H	-1.174654084	-3.531735252	1.598187117
O	4.875291352	-0.963333071	3.186660228
H	3.977214287	-1.156588084	2.929736212
H	5.355607385	-1.780278130	3.151695228
O	0.250223018	-3.376738241	3.022790216
H	0.891209064	-2.700111196	2.824264201
H	0.725182052	-4.087664295	3.431151246

LIIC path connecting S_i/T₁ and T1-MIN

Coord_1

C	-0.533673038	-0.207645014	0.062313002
N	0.262369017	-0.902803063	0.904136065
C	1.554121109	-0.633366047	1.254824088
C	1.454543107	0.858796063	-0.585176040
N	0.063997003	0.754815052	-0.570179040
N	2.098345148	0.418020028	0.582824043
H	3.074295223	0.610300042	0.724124052
N	-1.857491134	-0.469087034	0.015601003
H	-2.093587152	-1.389462100	0.341863023

H	-2.289872165	-0.216321018	-0.855486060
H	1.854996132	1.752325125	-1.033960072
O	2.134961155	-1.274335091	2.105551151
O	-2.764036200	0.430891031	-2.804599202
H	-2.478059178	-0.035569003	-3.578125258
H	-2.418954175	1.316614094	-2.868257209
O	-1.347239095	2.921258211	-2.297742168
H	-1.714106124	3.688796266	-1.877729137
H	-0.913591066	2.413792173	-1.621395117
O	4.918200356	1.125437081	1.243343090
H	5.121926368	1.993323145	1.564308110
H	5.130001370	0.507962036	1.940628140
O	-1.808420131	-3.475823251	0.887045064
H	-2.432870177	-4.176843303	1.015764075
H	-1.174654084	-3.531735252	1.598187117
O	4.875291352	-0.963333071	3.186660228
H	3.977214287	-1.156588084	2.929736212
H	5.355607385	-1.780278130	3.151695228
O	0.250223018	-3.376738241	3.022790216
H	0.891209064	-2.700111196	2.824264201
H	0.725182052	-4.087664295	3.431151246

Coord_2

C	-0.520863038	-0.205488014	0.067003005
N	0.275749020	-0.916616065	0.906960067
C	1.571987112	-0.631112043	1.248052090
C	1.458436105	0.871256060	-0.585222041
N	0.068066006	0.755778054	-0.576022041
N	2.111669154	0.416094029	0.570377042
H	3.084439223	0.620636043	0.715845053
N	-1.849118132	-0.469409034	0.028090004
H	-2.086896150	-1.395668100	0.340953024
H	-2.291320163	-0.208070012	-0.835775059
H	1.853594135	1.771986129	-1.023908075
O	2.151991154	-1.269781092	2.104711151
O	-2.780884198	0.432419031	-2.792311198
H	-2.494422180	-0.037532002	-3.563522257
H	-2.431530173	1.315830097	-2.857419204
O	-1.347031096	2.910094211	-2.293469168
H	-1.707606124	3.671753266	-1.857798131
H	-0.905301065	2.391654170	-1.630140115
O	4.923993355	1.134131082	1.241753087
H	5.134345370	2.001977145	1.558562113
H	5.142372370	0.516724036	1.936991142
O	-1.826164132	-3.492286252	0.863734060
H	-2.427318176	-4.219176303	0.955856066
H	-1.195094084	-3.552245257	1.573234113

O	4.899484352	-0.956812067	3.184171227
H	4.001859288	-1.156424081	2.931542210
H	5.383685387	-1.771757128	3.155159227
O	0.227020014	-3.377032241	2.997390216
H	0.851637063	-2.690092194	2.801252204
H	0.639156046	-4.046207289	3.528119257

Coord_3

C	-0.508000036	-0.203962015	0.070604003
N	0.288499022	-0.931747068	0.908288064
C	1.588208115	-0.630198043	1.240170090
C	1.461792105	0.883096063	-0.585200043
N	0.071897006	0.756082056	-0.582375041
N	2.123670153	0.413509030	0.558069041
H	3.092970222	0.630269043	0.708545053
N	-1.839885132	-0.470245033	0.039908003
H	-2.078715149	-1.401654100	0.340545023
H	-2.291638167	-0.200011013	-0.816442061
H	1.851721134	1.791101128	-1.013149071
O	2.167756159	-1.266801089	2.101869151
O	-2.796549199	0.433706032	-2.780317200
H	-2.509367183	-0.039707005	-3.549118253
H	-2.442945177	1.314927093	-2.846716203
O	-1.346079096	2.898819206	-2.288671165
H	-1.700189122	3.654390262	-1.837569135
H	-0.897384065	2.369146171	-1.638417119
O	4.927771352	1.143346085	1.241236091
H	5.144070373	2.011150147	1.554158110
H	5.153156372	0.525950040	1.934173140
O	-1.843323133	-3.507312251	0.843456062
H	-2.422227173	-4.255564309	0.902244066
H	-1.213732088	-3.571708259	1.551003112
O	4.923095357	-0.950410070	3.181880228
H	4.026135289	-1.156876083	2.933431214
H	5.411742391	-1.762941125	3.158507226
O	0.206808015	-3.381122241	2.974738213
H	0.817808058	-2.687473195	2.775010198
H	0.548872041	-3.993133288	3.614303259

Coord_4

C	-0.495250034	-0.202750014	0.073150007
N	0.300308020	-0.947855070	0.908246063
C	1.602524116	-0.630441047	1.231292089
C	1.464548107	0.894297062	-0.585224041
N	0.075401006	0.755925054	-0.589320043
N	2.134267155	0.410253029	0.545815037
H	3.099828221	0.639033044	0.702122053

N	-1.829964133	-0.471153032	0.051029001
H	-2.069141147	-1.407044104	0.340533026
H	-2.291000164	-0.191720012	-0.797504056
H	1.849438131	1.809536129	-1.001888073
O	2.182103159	-1.265006093	2.097254149
O	-2.811351202	0.434906031	-2.768670200
H	-2.523277183	-0.042021002	-3.534940256
H	-2.453452177	1.314027094	-2.836294205
O	-1.344466095	2.887523209	-2.283669165
H	-1.691905122	3.636856259	-1.817422129
H	-0.889888063	2.346416167	-1.646477118
O	4.929553357	1.152632082	1.241684088
H	5.151272369	2.020409146	1.550880111
H	5.162236371	0.535254040	1.932154139
O	-1.859255136	-3.520513254	0.825967061
H	-2.416977174	-4.286509308	0.854400061
H	-1.230171090	-3.589705259	1.531453109
O	4.945697358	-0.944280065	3.179956230
H	4.049595294	-1.157965082	2.935562210
H	5.439195392	-1.754076125	3.162034229
O	0.189730015	-3.389469245	2.955334214
H	0.789860059	-2.692030194	2.747629197
H	0.456479032	-3.929905285	3.689077264

Coord_5

C	-0.482757032	-0.201559016	0.074655003
N	0.310884024	-0.964632069	0.906933064
C	1.614693119	-0.631697043	1.221504088
C	1.466660107	0.904856064	-0.585397040
N	0.078505006	0.755497055	-0.596939041
N	2.143383154	0.406303027	0.533530039
H	3.104963225	0.646752046	0.696480049
N	-1.819501129	-0.471735032	0.061416005
H	-2.058223146	-1.411487102	0.340813025
H	-2.289559167	-0.182808011	-0.778986053
H	1.846822132	1.827187132	-0.990304071
O	2.194844160	-1.264086092	2.091067151
O	-2.825605205	0.436167029	-2.757407196
H	-2.536525184	-0.044396003	-3.521004252
H	-2.463315178	1.313251093	-2.826275202
O	-1.342307099	2.876292205	-2.278730163
H	-1.682843121	3.619285262	-1.797674129
H	-0.882886064	2.323602166	-1.654534117
O	4.929358355	1.161567086	1.242990092
H	5.156103371	2.029343145	1.548531114
H	5.169514374	0.544269040	1.930904137
O	-1.873261135	-3.531540255	0.811045056

H	-2.410721172	-4.312451313	0.811778056
H	-1.243933091	-3.605852262	1.514549108
O	4.966924357	-0.938595067	3.178532230
H	4.071853293	-1.159749082	2.938066214
H	5.465539392	-1.745414123	3.165982230
O	0.175968014	-3.402529244	2.939679209
H	0.767758055	-2.703568195	2.720897194
H	0.363598026	-3.857648280	3.752061269

Coord_6

C	-0.470656034	-0.200098015	0.075098004
N	0.319917022	-0.981785069	0.904413063
C	1.624451115	-0.633860045	1.210862085
C	1.468093108	0.914770067	-0.585831045
N	0.081141007	0.754992056	-0.605334042
N	2.150927153	0.401608029	0.521135035
H	3.108315224	0.653227049	0.691536052
N	-1.808616128	-0.471595033	0.071014005
H	-2.045949145	-1.414622102	0.341293025
H	-2.287455163	-0.172892013	-0.760919053
H	1.843972132	1.843966131	-0.978562073
O	2.205708158	-1.263796092	2.083483152
O	-2.839649204	0.437633030	-2.746553199
H	-2.549511183	-0.046747005	-3.507319252
H	-2.472824176	1.312716095	-2.816764204
O	-1.339751099	2.865212207	-2.274114166
H	-1.673129120	3.601809258	-1.778619128
H	-0.876477061	2.300835167	-1.662794119
O	4.927182357	1.169726084	1.245073092
H	5.158682369	2.037527146	1.546952112
H	5.174874373	0.552609038	1.930416141
O	-1.884521138	-3.540026253	0.798554060
H	-2.402351175	-4.333710310	0.773919054
H	-1.254376092	-3.619735259	1.500320108
O	4.986402360	-0.933572068	3.177746227
H	4.092514294	-1.162334086	2.941074211
H	5.490276396	-1.737247125	3.170585226
O	0.165841012	-3.420904247	2.928340211
H	0.751422052	-2.721999195	2.696375194
H	0.271483021	-3.777082272	3.802784273

Coord_7

C	-0.459091035	-0.198043014	0.074403004
N	0.327024026	-0.999009074	0.900695064
C	1.631444119	-0.636861046	1.199387088
C	1.468815107	0.924037067	-0.586660043
N	0.083241005	0.754624056	-0.614662045

N	2.156755156	0.396088028	0.508543035
H	3.109775224	0.658210046	0.687225052
N	-1.797408127	-0.470298035	0.079739005
H	-2.032221144	-1.416012102	0.341918026
H	-2.284823163	-0.161558010	-0.743355052
H	1.841019132	1.859780133	-0.966843072
O	2.214273162	-1.263946093	2.074645152
O	-2.853877204	0.439462030	-2.736124195
H	-2.562711186	-0.048979006	-3.493891252
H	-2.482325177	1.312555093	-2.807874201
O	-1.336987095	2.854377207	-2.270113162
H	-1.662920121	3.584572256	-1.760583127
H	-0.870793062	2.278253163	-1.671504122
O	4.922972355	1.176625084	1.247905090
H	5.159079374	2.044473148	1.546043113
H	5.178131374	0.559821041	1.930732139
O	-1.891992136	-3.545499258	0.788532057
H	-2.390431172	-4.350420315	0.740583052
H	-1.260574091	-3.630836260	1.488961107
O	5.003658360	-0.929507066	3.177782227
H	4.111080298	-1.165898084	2.944750214
H	5.512799397	-1.729949125	3.176130231
O	0.159930012	-3.445516249	2.922028211
H	0.740844053	-2.747451197	2.675483192
H	0.181249013	-3.688469266	3.840288277

Coord_8

C	-0.448242034	-0.194978014	0.072378007
N	0.331672022	-1.015947075	0.895700065
C	1.635132119	-0.640659047	1.187041086
C	1.468783108	0.932649067	-0.588082043
N	0.084721008	0.754663056	-0.625186047
N	2.160622156	0.389622027	0.495649034
H	3.109142222	0.661365048	0.683505047
N	-1.785949127	-0.467297034	0.087452007
H	-2.016789145	-1.415056101	0.342699023
H	-2.281798163	-0.148303009	-0.726383051
H	1.838141133	1.874523133	-0.955376071
O	2.219848161	-1.264396089	2.064641151
O	-2.868793207	0.441850033	-2.726145198
H	-2.576740183	-0.050969003	-3.480734249
H	-2.492265179	1.312936095	-2.799756204
O	-1.334266097	2.843912203	-2.267128163
H	-1.652418117	3.567757257	-1.743999125
H	-0.866016063	2.256033163	-1.681014120
O	4.916569352	1.181643087	1.251553090
H	5.157275372	2.049543147	1.545810111

H	5.178953372	0.565302042	1.932007139
O	-1.894228138	-3.547254253	0.781353058
H	-2.373028173	-4.362406312	0.711951049
H	-1.261120091	-3.638408262	1.480997106
O	5.017963359	-0.926849067	3.178933230
H	4.126797296	-1.170740083	2.949334212
H	5.532225398	-1.724066124	3.183036227
O	0.159275012	-3.477865251	2.921764210
H	0.736238052	-2.780440202	2.659600191
H	0.094232006	-3.591542261	3.862563279

Coord_9

C	-0.438372031	-0.190285016	0.068623007
N	0.333015026	-1.032091077	0.889174066
C	1.634586119	-0.645237049	1.173680086
C	1.467918104	0.940611068	-0.590428044
N	0.085457009	0.755507057	-0.637391044
N	2.162072155	0.382027026	0.482302035
H	3.106017224	0.662203048	0.680366047
N	-1.774266127	-0.461806032	0.093899005
H	-1.999121144	-1.410826102	0.343774025
H	-2.278524165	-0.132434010	-0.710178051
H	1.835602130	1.888060138	-0.944512067
O	2.221232160	-1.265057090	2.053461149
O	-2.885112208	0.445082030	-2.716667195
H	-2.592480185	-0.052536003	-3.467892250
H	-2.503283179	1.314108096	-2.792653200
O	-1.331952095	2.834017203	-2.265796161
H	-1.641895121	3.551646255	-1.729549125
H	-0.862417065	2.234435159	-1.691902122
O	4.907612355	1.183863086	1.256270091
H	5.153098369	2.051779149	1.546462110
H	5.176686371	0.568131039	1.934614141
O	-1.888991135	-3.544095255	0.778045055
H	-2.347353170	-4.368946313	0.689012051
H	-1.253690093	-3.641230264	1.477636105
O	5.028028364	-0.926352064	3.181719231
H	4.138338297	-1.177393084	2.955218214
H	5.547040398	-1.720492124	3.192004230
O	0.165758010	-3.520483255	2.929186212
H	0.738274051	-2.822201204	2.650228192
H	0.012659999	-3.485381251	3.865458280

Coord_10

C	-0.423898028	-0.152036010	0.053306003
N	0.319811022	-0.996880072	0.905004064
C	1.620508115	-0.606153044	1.180635083

C	1.489371108	0.936257066	-0.624707046
N	0.107005006	0.759349053	-0.687253050
N	2.169131157	0.388648029	0.461328031
H	3.110036225	0.672011047	0.668896050
N	-1.759399125	-0.405889031	0.087894007
H	-1.987531141	-1.344138095	0.363768025
H	-2.262516162	-0.086644006	-0.720380054
H	1.870221133	1.872892134	-0.993036070
O	2.195130159	-1.198825086	2.086624153
O	-2.870002208	0.416966028	-2.755116198
H	-2.577399183	-0.113193009	-3.483789253
H	-2.472259178	1.276549089	-2.859336207
O	-1.273743090	2.788246202	-2.379464170
H	-1.571062111	3.520601251	-1.856362135
H	-0.814580060	2.190624157	-1.794270127
O	4.907009353	1.193007083	1.250597089
H	5.165241373	2.066870151	1.510222110
H	5.169779370	0.597335041	1.948988140
O	-1.908706136	-3.461944250	0.868896062
H	-2.353677172	-4.294625310	0.785986058
H	-1.276836094	-3.549353256	1.577374116
O	5.005178363	-0.855862061	3.243423235
H	4.115876295	-1.110795080	3.020890216
H	5.519218396	-1.651977117	3.290351235
O	0.129721008	-3.457999249	3.051432221
H	0.705336053	-2.771724198	2.735364196
H	-0.116294008	-3.217004231	3.935135281

LIIC path connecting T1-MIN and S₁/T₁/S₀-III

Coord_1

C	-0.423898028	-0.152036010	0.053306003
N	0.319811022	-0.996880072	0.905004064
C	1.620508115	-0.606153044	1.180635083
C	1.489371108	0.936257066	-0.624707046
N	0.107005006	0.759349053	-0.687253050
N	2.169131157	0.388648029	0.461328031
H	3.110036225	0.672011047	0.668896050
N	-1.759399125	-0.405889031	0.087894007
H	-1.987531141	-1.344138095	0.363768025
H	-2.262516162	-0.086644006	-0.720380054
H	1.870221133	1.872892134	-0.993036070
O	2.195130159	-1.198825086	2.086624153
O	-2.870002208	0.416966028	-2.755116198
H	-2.577399183	-0.113193009	-3.483789253
H	-2.472259178	1.276549089	-2.859336207
O	-1.273743090	2.788246202	-2.379464170
H	-1.571062111	3.520601251	-1.856362135

H	-0.814580060	2.190624157	-1.794270127
O	4.907009353	1.193007083	1.250597089
H	5.165241373	2.066870151	1.510222110
H	5.169779370	0.597335041	1.948988140
O	-1.908706136	-3.461944250	0.868896062
H	-2.353677172	-4.294625310	0.785986058
H	-1.276836094	-3.549353256	1.577374116
O	5.005178363	-0.855862061	3.243423235
H	4.115876295	-1.110795080	3.020890216
H	5.519218396	-1.651977117	3.290351235
O	0.129721008	-3.457999249	3.051432221
H	0.705336053	-2.771724198	2.735364196
H	-0.116294008	-3.217004231	3.935135281

Coord_2

C	-0.408578029	-0.160743013	0.036891005
N	0.352191023	-1.021099076	0.866303062
C	1.635060119	-0.594855041	1.179596086
C	1.505070109	0.914719065	-0.644526046
N	0.113611006	0.756028053	-0.699049052
N	2.175090158	0.415260030	0.473611034
H	3.115571223	0.698910053	0.682497049
N	-1.743235125	-0.405063027	0.095411007
H	-1.973708142	-1.347601100	0.353121026
H	-2.261103163	-0.064820006	-0.695281050
H	1.898242138	1.827834131	-1.056086074
O	2.203509157	-1.171606086	2.097954150
O	-2.883745206	0.409544032	-2.736006199
H	-2.588242184	-0.119382006	-3.464392250
H	-2.487413180	1.269977089	-2.838855206
O	-1.291310092	2.784350203	-2.365620168
H	-1.580293116	3.519523254	-1.841878130
H	-0.820074058	2.190811157	-1.785505126
O	4.920699353	1.201851085	1.255222093
H	5.179234375	2.074088150	1.520027108
H	5.176926374	0.602736046	1.953002140
O	-1.914981136	-3.459504251	0.857520064
H	-2.357684171	-4.292068310	0.762419054
H	-1.286410091	-3.553460253	1.568073111
O	4.994001362	-0.853448061	3.243248231
H	4.100493297	-1.098345079	3.026593218
H	5.498933397	-1.655448117	3.288643236
O	0.107837010	-3.459482247	3.052042219
H	0.697803051	-2.778078198	2.751994200
H	-0.146818010	-3.226318232	3.935436283

Coord_3

C	-0.394832031	-0.168931010	0.019946003
N	0.382752026	-1.044485075	0.825974062
C	1.645996117	-0.585985041	1.179336085
C	1.520741111	0.888777066	-0.663156049
N	0.120279009	0.752226052	-0.711276052
N	2.177912155	0.438557032	0.486432036
H	3.117992225	0.722549051	0.696440049
N	-1.728160125	-0.404050029	0.105021009
H	-1.961009142	-1.350365098	0.345475023
H	-2.261250163	-0.043282005	-0.666601046
H	1.928738141	1.774949130	-1.116736079
O	2.204669161	-1.148865081	2.110518151
O	-2.896842211	0.405261030	-2.717998197
H	-2.599085185	-0.122552011	-3.446263246
H	-2.500901178	1.266099093	-2.819218205
O	-1.305516093	2.781636201	-2.352181172
H	-1.585166113	3.519891254	-1.827775133
H	-0.822908061	2.191559160	-1.777534129
O	4.930988353	1.210435086	1.257680089
H	5.189071373	2.081785150	1.525872109
H	5.181862375	0.609499042	1.955746141
O	-1.921158137	-3.456583250	0.847341059
H	-2.361587170	-4.288947307	0.740791056
H	-1.294173094	-3.557243257	1.558354115
O	4.983123361	-0.847316060	3.244581234
H	4.085645293	-1.083465080	3.034967220
H	5.479778393	-1.654483120	3.289498238
O	0.090571004	-3.461244249	3.049500221
H	0.694099048	-2.785060200	2.764677197
H	-0.170956013	-3.236060231	3.932994283

Coord_4

C	-0.382658028	-0.176715012	0.002432998
N	0.411485027	-1.067174078	0.783845054
C	1.653298118	-0.579734044	1.179704086
C	1.536234109	0.858067064	-0.680619052
N	0.127022008	0.747877051	-0.723963050
N	2.177581155	0.458369031	0.499588039
H	3.117289224	0.742797055	0.710445053
N	-1.714033124	-0.403031029	0.116495006
H	-1.949356141	-1.352687096	0.340423026
H	-2.262645164	-0.022106004	-0.634551045
H	1.961527143	1.713734123	-1.174812086
O	2.198667159	-1.131023081	2.123949151
O	-2.909453208	0.404522028	-2.701042194
H	-2.610162187	-0.122291010	-3.429394245
H	-2.512796182	1.265283091	-2.800341204

O	-1.316256095	2.780334198	-2.339014168
H	-1.585482117	3.521891253	-1.813865132
H	-0.823010060	2.192976159	-1.770277125
O	4.937737358	1.218905087	1.257975090
H	5.194437373	2.090169148	1.527807109
H	5.184480374	0.617792043	1.957270140
O	-1.927023141	-3.453370250	0.838364059
H	-2.365148168	-4.285494309	0.721124051
H	-1.300008094	-3.560740256	1.548342113
O	4.972538356	-0.837408058	3.247470235
H	4.071380293	-1.066229079	3.045913220
H	5.461902393	-1.648967119	3.293058236
O	0.077851006	-3.463060248	3.044184218
H	0.694213049	-2.792434200	2.773729198
H	-0.188935016	-3.245942236	3.928163281

Coord_5

C	-0.372087024	-0.184148015	-0.015634002
N	0.438346033	-1.089213078	0.739817052
C	1.656885119	-0.576260043	1.180605084
C	1.551337113	0.822176061	-0.696890051
N	0.133844008	0.742944056	-0.737096054
N	2.174043155	0.474526035	0.512887035
H	3.113424224	0.759504054	0.724218050
N	-1.700743123	-0.402212027	0.129600012
H	-1.938643138	-1.354851098	0.337554023
H	-2.264984165	-0.001444998	-0.599370045
H	1.996342143	1.643587117	-1.230095090
O	2.185477156	-1.118449078	2.137927152
O	-2.921724209	0.407773029	-2.685028195
H	-2.621711190	-0.118173011	-3.413704245
H	-2.523144180	1.267926093	-2.782100200
O	-1.323374095	2.780676199	-2.325991168
H	-1.580969113	3.525724253	-1.799988131
H	-0.820272060	2.195179156	-1.763646127
O	4.940800358	1.227328091	1.256063093
H	5.195040376	2.099348151	1.525805110
H	5.184639376	0.627714043	1.957578142
O	-1.932222138	-3.450089251	0.830537062
H	-2.367920173	-4.282011307	0.703361052
H	-1.303680092	-3.563988256	1.538116112
O	4.962154358	-0.823670061	3.251935237
H	4.057647292	-1.046685076	3.059317221
H	5.445336394	-1.638804117	3.299453237
O	0.069658004	-3.464633248	3.036443217
H	0.698140052	-2.799831204	2.779477200
H	-0.200963014	-3.255633233	3.921251284

Coord_6

C	-0.363181024	-0.191223014	-0.034175002
N	0.463247034	-1.110561077	0.693886049
C	1.656627119	-0.575686039	1.181997085
C	1.565757114	0.780638055	-0.711878049
N	0.140746008	0.737424054	-0.750597054
N	2.167213154	0.486856034	0.526150038
H	3.106343224	0.772497055	0.737445052
N	-1.688218122	-0.401834030	0.144073009
H	-1.928738141	-1.357184097	0.336400025
H	-2.267976165	0.018463000	-0.561380039
H	2.032804149	1.563798110	-1.282307094
O	2.165017158	-1.111454080	2.152171153
O	-2.933789213	0.415506028	-2.669764194
H	-2.633962188	-0.109747006	-3.399014243
H	-2.531959183	1.274452092	-2.764315198
O	-1.326664096	2.782905200	-2.312967169
H	-1.571286111	3.531608254	-1.785992128
H	-0.814548061	2.198297158	-1.757524128
O	4.940033357	1.235671089	1.251834088
H	5.190619375	2.109317152	1.519737109
H	5.182177373	0.639294044	1.956609139
O	-1.936230137	-3.447024251	0.823720058
H	-2.369188172	-4.278900306	0.687322050
H	-1.304816092	-3.567032258	1.527692109
O	4.951799354	-0.806056057	3.257958237
H	4.044305289	-1.024843073	3.075048221
H	5.429998392	-1.623912117	3.308783240
O	0.065997007	-3.465548249	3.026632218
H	0.705838052	-2.806695205	2.782311198
H	-0.207289016	-3.264719233	3.912550282

Coord_7

C	-0.356034025	-0.197881017	-0.053030006
N	0.486055034	-1.131107083	0.646170047
C	1.652350118	-0.578097040	1.183899086
C	1.579102112	0.732932054	-0.725413054
N	0.147723009	0.731348052	-0.764309053
N	2.156992154	0.495182035	0.539209037
H	3.095991221	0.781576059	0.749781052
N	-1.676447119	-0.402193029	0.159585010
H	-1.919507136	-1.360086100	0.336387023
H	-2.271352162	0.037267001	-0.521049039
H	2.070376146	1.473540104	-1.331093098
O	2.137167152	-1.110279079	2.166440158
O	-2.945759213	0.428268032	-2.654949189

H	-2.647140189	-0.096525005	-3.385024246
H	-2.539223183	1.285322091	-2.746718197
O	-1.325867097	2.787273198	-2.299758164
H	-1.556025110	3.539776254	-1.771697130
H	-0.805657058	2.202473160	-1.751742126
O	4.935309355	1.243794092	1.245091090
H	5.180971373	2.119944153	1.509354111
H	5.176921373	0.652472045	1.954220142
O	-1.938316138	-3.444545246	0.817631058
H	-2.367901170	-4.276705310	0.672649049
H	-1.302890094	-3.569920259	1.517011110
O	4.941237357	-0.784524057	3.265463235
H	4.031137290	-1.000684073	3.092944223
H	5.415704389	-1.604227115	3.321102238
O	0.066859005	-3.465225249	3.015148220
H	0.717182051	-2.812204204	2.782741203
H	-0.208282017	-3.272655235	3.902362281

Coord_8

C	-0.350773024	-0.204029014	-0.071947008
N	0.506592038	-1.150690081	0.596925045
C	1.643846118	-0.583553042	1.186395088
C	1.590841116	0.678487049	-0.737216051
N	0.154767009	0.724776051	-0.777963059
N	2.143269154	0.499324037	0.551908042
H	3.082320223	0.786504059	0.760848053
N	-1.665517122	-0.403671027	0.175690011
H	-1.910830137	-1.364062100	0.336749023
H	-2.274888162	0.054477004	-0.479082034
H	2.108302153	1.371866099	-1.375985098
O	2.101797152	-1.115091078	2.180531159
O	-2.957715210	0.446662032	-2.640153192
H	-2.661445194	-0.077973008	-3.371300241
H	-2.544880183	1.301037095	-2.728928194
O	-1.320680096	2.794046201	-2.286088166
H	-1.534718111	3.550465258	-1.756850125
H	-0.793387057	2.207863159	-1.746036124
O	4.926529357	1.251426093	1.235538091
H	5.165961372	2.130938154	1.494273110
H	5.168705373	0.667075046	1.950166142
O	-1.937486139	-3.443142249	0.811803060
H	-2.362570170	-4.276157310	0.658751045
H	-1.297182091	-3.572691258	1.505918110
O	4.930177357	-0.759069055	3.274298236
H	4.017863291	-0.974171071	3.112792223
H	5.402173390	-1.579723112	3.336395238
O	0.072188005	-3.462814249	3.002475218

H	0.731914054	-2.815140201	2.781467198
H	-0.204497013	-3.278660238	3.891032279

Coord_9

C	-0.347563024	-0.209566018	-0.090586006
N	0.524616037	-1.169141084	0.546559039
C	1.630875116	-0.592109045	1.189625085
C	1.600263117	0.616682047	-0.746882055
N	0.161856011	0.717786054	-0.791149055
N	2.125919151	0.499076038	0.564111039
H	3.065287219	0.786979059	0.770239055
N	-1.655655121	-0.406776027	0.191756012
H	-1.902639135	-1.369782098	0.336408026
H	-2.278433162	0.069420006	-0.436540030
H	2.145527153	1.257727091	-1.416373102
O	2.058776147	-1.126000083	2.194281158
O	-2.969701213	0.471362036	-2.624794187
H	-2.677050192	-0.053476002	-3.357256242
H	-2.548833185	1.322150097	-2.710410198
O	-1.310769093	2.803505202	-2.271530161
H	-1.506856109	3.563909255	-1.741044125
H	-0.777509056	2.214634161	-1.739994126
O	4.913625354	1.258117089	1.222778087
H	5.145533373	2.141811154	1.473980104
H	5.157369369	0.682773052	1.944088139
O	-1.932374139	-3.443461247	0.805516059
H	-2.351071169	-4.278246306	0.644751047
H	-1.286689094	-3.575338256	1.494146107
O	4.918285353	-0.729775051	3.284200237
H	4.004148287	-0.945304066	3.134306225
H	5.389035390	-1.550470109	3.354531243
O	0.081872007	-3.457006248	2.989243215
H	0.749585055	-2.813648202	2.779460198
H	-0.196752012	-3.281525236	3.878986279

Coord_10

C	-0.279066020	-0.221724018	-0.067443005
N	0.576741039	-1.195788084	0.576110043
C	1.644928116	-0.617284044	1.285418095
C	1.700646120	0.491885033	-0.685399051
N	0.267707018	0.679219050	-0.769785053
N	2.169191155	0.458764035	0.655589047
H	3.109632225	0.735103051	0.871959062
N	-1.589551114	-0.390287028	0.223329018
H	-1.856962132	-1.348902098	0.364873026
H	-2.202189156	0.101146008	-0.402471027
H	2.300010164	1.050128078	-1.382207101

O	2.008146145	-1.141668085	2.318607167
O	-2.846417207	0.488158038	-2.638677189
H	-2.552359183	-0.057574003	-3.355138241
H	-2.399043172	1.324826094	-2.729082196
O	-1.127765080	2.778486199	-2.297183166
H	-1.301762094	3.556863255	-1.785377129
H	-0.611774044	2.187477155	-1.750850129
O	4.959872355	1.192614085	1.331232097
H	5.193482372	2.082156151	1.559083115
H	5.180235372	0.639821047	2.077220149
O	-1.929670138	-3.406028244	0.871079061
H	-2.349978170	-4.240188307	0.711322053
H	-1.295928095	-3.534091255	1.571384115
O	4.888650352	-0.722688050	3.459663247
H	3.972543287	-0.927002068	3.306458237
H	5.342839386	-1.548621111	3.567457256
O	0.039307000	-3.393977243	3.092942223
H	0.728402053	-2.769150200	2.896238208
H	-0.258807019	-3.203881233	3.973354288

Relaxation pathway II'

LIIC path connecting S2-MIN and S₁/S₀-I

Coord_1

C	-0.373591026	-0.216509014	0.096070008
N	0.391908030	-1.007749071	0.993653070
C	1.592742116	-0.571826041	1.213374089
C	1.499077108	0.898384062	-0.590315044
N	0.118952008	0.714147050	-0.641966046
N	2.155088153	0.470830033	0.562369040
H	3.111154223	0.715774053	0.752050053
N	-1.697154121	-0.504147038	0.118751010
H	-1.929674139	-1.434006103	0.412078029
H	-2.207295161	-0.190024015	-0.686825052
H	1.899777138	1.775449129	-1.067684078
O	2.324976169	-1.146852085	2.127243153
O	-2.842168205	0.383047026	-2.740070196
H	-2.509548182	-0.156216013	-3.444381249
H	-2.414772172	1.231371090	-2.817512201
O	-1.196135087	2.720983196	-2.330915168
H	-1.509102106	3.451587251	-1.814755129
H	-0.772810058	2.110702152	-1.728699123
O	4.914020353	1.165513081	1.289280094
H	5.203465375	2.049216147	1.471849108
H	5.220375377	0.610337042	2.002503142
O	-2.284770166	-3.608108261	0.685903050
H	-2.832611205	-4.362884312	0.518890038

H	-1.676933121	-3.839280279	1.382490100
O	5.237757378	-0.776232056	3.396705247
H	4.363718317	-1.136281081	3.308363238
H	5.833102422	-1.512325108	3.468175248
O	-0.184234012	-3.475678252	2.664271191
H	0.055879006	-2.686603196	2.188077158
H	-0.394389030	-3.202874230	3.547525255

Coord_2

C	-0.378987025	-0.212114017	0.085153007
N	0.392769028	-1.010208073	0.980517070
C	1.584290113	-0.563294042	1.201168087
C	1.500276107	0.885860061	-0.611243046
N	0.111122010	0.717608049	-0.650824049
N	2.150018153	0.477785036	0.553915042
H	3.103501225	0.726506053	0.749918056
N	-1.704949125	-0.493596038	0.126166011
H	-1.933724139	-1.427093100	0.410633031
H	-2.220710159	-0.177294011	-0.675050048
H	1.902910137	1.758144128	-1.096148078
O	2.328958170	-1.135603084	2.122764154
O	-2.848951204	0.387391026	-2.745518198
H	-2.499977181	-0.155392010	-3.439086248
H	-2.419473176	1.235172091	-2.817744203
O	-1.201191085	2.724172198	-2.332369167
H	-1.513813107	3.455160250	-1.816596131
H	-0.777388055	2.114086150	-1.729690124
O	4.907062355	1.162555081	1.301744091
H	5.204306375	2.044846149	1.478921106
H	5.211213377	0.608281045	2.016274144
O	-2.279089162	-3.614445259	0.689151050
H	-2.823064202	-4.372199314	0.522922035
H	-1.667467119	-3.843146278	1.383023097
O	5.253793381	-0.786649059	3.404606244
H	4.379679313	-1.155082082	3.365637240
H	5.858439423	-1.516550107	3.458379252
O	-0.183563015	-3.464321251	2.667054192
H	0.046356001	-2.680166194	2.179724158
H	-0.418998032	-3.184000229	3.537560255

Coord_3

C	-0.384389030	-0.207881017	0.074574007
N	0.393564027	-1.012776075	0.967717072
C	1.575597112	-0.554902042	1.189644088
C	1.501346109	0.872770063	-0.631291043
N	0.103493010	0.720916053	-0.659207048
N	2.144502152	0.484720036	0.546222038

H	3.095238223	0.737624052	0.748558055
N	-1.712482122	-0.483296036	0.133932010
H	-1.937640140	-1.420364104	0.409306029
H	-2.233705159	-0.164747012	-0.662906050
H	1.905998135	1.740169125	-1.123679080
O	2.332509166	-1.124247083	2.119169152
O	-2.855079203	0.391573029	-2.751161196
H	-2.489970180	-0.154714012	-3.433544249
H	-2.423483176	1.238759087	-2.818035203
O	-1.205701088	2.727178195	-2.333619168
H	-1.518077111	3.458546249	-1.818286133
H	-0.781511054	2.117298150	-1.730404122
O	4.899796355	1.159796083	1.313448095
H	5.204975377	2.040497148	1.485116105
H	5.202262375	0.606228044	2.028963148
O	-2.274618165	-3.620821263	0.691514049
H	-2.815207200	-4.381098318	0.525689040
H	-1.659420122	-3.847742278	1.382589098
O	5.269935377	-0.796170058	3.411802245
H	4.398437319	-1.172551086	3.422651246
H	5.883183423	-1.519868112	3.447867246
O	-0.182892013	-3.452963249	2.669836193
H	0.036833001	-2.673729192	2.171371154
H	-0.443608034	-3.165125228	3.527595255

Coord_4

C	-0.389860030	-0.203796017	0.064360003
N	0.394189028	-1.015425073	0.955336070
C	1.566546112	-0.546614042	1.178924084
C	1.502259109	0.859102060	-0.650357045
N	0.096037008	0.724071050	-0.667082047
N	2.138444152	0.491656037	0.539411040
H	3.086251221	0.749168053	0.748122055
N	-1.719822122	-0.473239033	0.142009012
H	-1.941509141	-1.413802099	0.408054027
H	-2.246310161	-0.152385013	-0.650471046
H	1.909044138	1.721497122	-1.150173085
O	2.335457170	-1.112721078	2.116644151
O	-2.860501206	0.395572027	-2.757082197
H	-2.479471176	-0.154221010	-3.427816249
H	-2.426748173	1.242107091	-2.818466202
O	-1.209622085	2.729979199	-2.334723170
H	-1.521867111	3.461732251	-1.819909130
H	-0.785161055	2.120323155	-1.730870126
O	4.892182351	1.157251085	1.324426094
H	5.205467374	2.036183147	1.490426108
H	5.193535375	0.604202041	2.040585145

O	-2.271451166	-3.627244263	0.692938049
H	-2.809119201	-4.389603318	0.527115040
H	-1.652910120	-3.853063277	1.381169098
O	5.286467382	-0.804830060	3.418257244
H	4.420354316	-1.188709085	3.479301253
H	5.907673423	-1.522291109	3.436499249
O	-0.182220011	-3.441605248	2.672618195
H	0.027310002	-2.667291190	2.163018154
H	-0.468217035	-3.146249227	3.517629254

Coord_5

C	-0.395473029	-0.199854012	0.054546003
N	0.394522028	-1.018134074	0.943463069
C	1.556999114	-0.538408037	1.169146084
C	1.502987109	0.844832060	-0.668315045
N	0.088720005	0.727067050	-0.674407050
N	2.131738154	0.498604033	0.533624037
H	3.076412223	0.761166057	0.748793052
N	-1.727052123	-0.463419033	0.150346009
H	-1.945429137	-1.407393101	0.406825029
H	-2.258562165	-0.140213011	-0.637834044
H	1.912054140	1.702089123	-1.175497084
O	2.337595168	-1.100976079	2.115397150
O	-2.865153209	0.399371028	-2.763377199
H	-2.468407176	-0.153948012	-3.421967248
H	-2.429196173	1.245193088	-2.819125202
O	-1.212892088	2.732548195	-2.335733168
H	-1.525141109	3.464704248	-1.821546129
H	-0.788314057	2.123144151	-1.731111124
O	4.884171354	1.154929081	1.334705098
H	5.205763375	2.031912147	1.494830106
H	5.185048372	0.602222045	2.051137146
O	-2.269704161	-3.633718259	0.693354051
H	-2.804903204	-4.397734317	0.527106039
H	-1.648088119	-3.859103280	1.378737100
O	5.303716380	-0.812631058	3.423926246
H	4.445857320	-1.203562085	3.535483255
H	5.932288426	-1.523788109	3.424121248
O	-0.181549014	-3.430247247	2.675401191
H	0.017787002	-2.660853193	2.154665155
H	-0.492826037	-3.127374226	3.507664254

Coord_6

C	-0.401312029	-0.196054016	0.045167003
N	0.394418029	-1.020895072	0.932203066
C	1.546793111	-0.530276038	1.160467085
C	1.503499109	0.829919062	-0.685014049

N	0.081508007	0.729890052	-0.681131046
N	2.124260154	0.505553036	0.529029037
H	3.065571223	0.773626054	0.750784055
N	-1.734273127	-0.453835035	0.158881013
H	-1.949523138	-1.401128103	0.405549029
H	-2.270509162	-0.128238010	-0.625104045
H	1.915042139	1.681892120	-1.199487086
O	2.338682167	-1.088981076	2.115664151
O	-2.868954204	0.402961030	-2.770160199
H	-2.456686175	-0.153922009	-3.416076245
H	-2.430740175	1.247999088	-2.820109202
O	-1.215435086	2.734863198	-2.336700171
H	-1.527842109	3.467452249	-1.823273131
H	-0.790935056	2.125740152	-1.731141123
O	4.875700353	1.152839085	1.344300097
H	5.205828374	2.027691148	1.498283109
H	5.176826370	0.600311043	2.060598147
O	-2.269525162	-3.640247264	0.692679049
H	-2.802691201	-4.405504317	0.525548040
H	-1.645141120	-3.865857280	1.375250097
O	5.322069385	-0.819536059	3.428752247
H	4.475463322	-1.217087088	3.591098260
H	5.957461430	-1.524277111	3.410567246
O	-0.180878012	-3.418889246	2.678183192
H	0.008264002	-2.654416191	2.146311155
H	-0.517435039	-3.108499224	3.497698254

Coord_7

C	-0.407477028	-0.192405016	0.036264004
N	0.393703026	-1.023716074	0.921669068
C	1.535737111	-0.522234036	1.153065081
C	1.503762110	0.814306058	-0.700270049
N	0.074365004	0.732517052	-0.687190052
N	2.115866154	0.512470038	0.525824038
H	3.053557222	0.786531057	0.754348053
N	-1.741611128	-0.444491029	0.167540009
H	-1.953936143	-1.395003099	0.404143032
H	-2.282212165	-0.116465007	-0.612406046
H	1.918032139	1.660829120	-1.221939087
O	2.338426167	-1.076736078	2.117714152
O	-2.871806205	0.406341028	-2.777561198
H	-2.444201174	-0.154161012	-3.410234245
H	-2.431269178	1.250519088	-2.821527201
O	-1.217149086	2.736902197	-2.337667168
H	-1.529890110	3.469962248	-1.825168131
H	-0.792975055	2.128090154	-1.730970125
O	4.866692349	1.150985081	1.353219099

H	5.205605373	2.023527148	1.500715107
H	5.168904370	0.598493044	2.068929148
O	-2.271101163	-3.646832261	0.690803052
H	-2.802659201	-4.412920318	0.522295040
H	-1.644310116	-3.873324278	1.370653098
O	5.341994385	-0.825455060	3.432671249
H	4.509804327	-1.229223091	3.646048264
H	5.983706431	-1.523608109	3.395661243
O	-0.180207015	-3.407531245	2.680965193
H	-0.001259003	-2.647978189	2.137958156
H	-0.542045040	-3.089624223	3.487732253

Coord_8

C	-0.414089029	-0.188931015	0.027879000
N	0.392166031	-1.026628073	0.911990067
C	1.523600108	-0.514328038	1.147146080
C	1.503741107	0.797905056	-0.713869052
N	0.067247003	0.734910055	-0.692507050
N	2.106391151	0.519288037	0.524242036
H	3.040170218	0.799823059	0.759780052
N	-1.749218125	-0.435393033	0.176233011
H	-1.958850141	-1.389015098	0.402503027
H	-2.293752166	-0.104897007	-0.599889046
H	1.921060139	1.638796116	-1.242607089
O	2.336481171	-1.064278076	2.121852154
O	-2.873589204	0.409528029	-2.785734203
H	-2.430822176	-0.154668011	-3.404547246
H	-2.430646177	1.252756090	-2.823501202
O	-1.217900089	2.738642195	-2.338674166
H	-1.531175111	3.472227249	-1.827300133
H	-0.794365056	2.130167154	-1.730597123
O	4.857046347	1.149367085	1.361457098
H	5.205010377	2.019426146	1.502028107
H	5.161321371	0.596793041	2.076068152
O	-2.274678163	-3.653476261	0.687585051
H	-2.805042203	-4.419981320	0.517160036
H	-1.645901119	-3.881507279	1.364864100
O	5.364053387	-0.830235060	3.435608247
H	4.549661328	-1.239849091	3.700242264
H	6.011635432	-1.521543111	3.379212245
O	-0.179535013	-3.396173244	2.683747194
H	-0.010782002	-2.641541192	2.129605151
H	-0.566654042	-3.070749222	3.477767253

Coord_9

C	-0.421290031	-0.185672014	0.020061004
N	0.389551027	-1.029690072	0.903306067

C	1.510107109	-0.506647035	1.142939084
C	1.503394110	0.780596054	-0.725554053
N	0.060110006	0.737012053	-0.696989049
N	2.095642153	0.525894038	0.524554039
H	3.025179219	0.813392058	0.767429055
N	-1.757280124	-0.426554032	0.184854012
H	-1.964487144	-1.383167097	0.400499027
H	-2.305227169	-0.093534005	-0.587727044
H	1.924174141	1.615649114	-1.261192090
O	2.332427170	-1.051696078	2.128423155
O	-2.874157207	0.412560030	-2.794854202
H	-2.416400175	-0.155429010	-3.399134244
H	-2.428705176	1.254730090	-2.826163202
O	-1.217516086	2.740065195	-2.339746168
H	-1.531543111	3.474240249	-1.829731131
H	-0.795015055	2.131940151	-1.730007123
O	4.846637351	1.147972083	1.369005097
H	5.203918377	2.015387148	1.502095106
H	5.154122370	0.595243044	2.081932150
O	-2.280568165	-3.660175264	0.682846052
H	-2.810145202	-4.426675317	0.509908037
H	-1.650303117	-3.890416280	1.357770098
O	5.388938387	-0.833634061	3.437484249
H	4.596003332	-1.248759092	3.753597269
H	6.041991436	-1.517733109	3.361021242
O	-0.178864011	-3.384815242	2.686529196
H	-0.020305002	-2.635103190	2.121252152
H	-0.591263044	-3.051874221	3.467801247

Coord_10

C	-0.412763027	-0.198008014	0.034189004
N	0.405097027	-1.056480078	0.906308063
C	1.516807107	-0.526772038	1.149285083
C	1.516957108	0.748820056	-0.716934052
N	0.067351003	0.727846052	-0.674833049
N	2.103976150	0.508137035	0.540272037
H	3.030796218	0.799438056	0.788131057
N	-1.749006126	-0.432124030	0.219997017
H	-1.954863140	-1.392721101	0.418584030
H	-2.303200166	-0.089682007	-0.543891038
H	1.940422142	1.581051114	-1.255276090
O	2.351911170	-1.075651080	2.137841155
O	-2.870726207	0.425988029	-2.766074199
H	-2.402418175	-0.142367011	-3.361889241
H	-2.421135174	1.266280093	-2.786699200
O	-1.206202086	2.744934198	-2.293296164

H	-1.517070108	3.476532248	-1.777719130
H	-0.783142058	2.131773154	-1.688415119
O	4.861567352	1.111179082	1.378857102
H	5.230761375	1.974148142	1.508285110
H	5.176342374	0.552358038	2.083569149
O	-2.275856164	-3.683598263	0.681468048
H	-2.807469200	-4.447300318	0.502444035
H	-1.641552119	-3.922996283	1.349164099
O	5.450944392	-0.887440063	3.423129247
H	4.684658339	-1.309065095	3.791900272
H	6.107292438	-1.564321112	3.317193237
O	-0.178674015	-3.374133244	2.689807195
H	-0.030319004	-2.629336189	2.113399151
H	-0.616389046	-3.033691220	3.458318248

LIIC path connecting S₁/S₀-I and S₀-MIN

Coord_1

C	-0.412763027	-0.198008014	0.034189004
N	0.405097027	-1.056480078	0.906308063
C	1.516807107	-0.526772038	1.149285083
C	1.516957108	0.748820056	-0.716934052
N	0.067351003	0.727846052	-0.674833049
N	2.103976150	0.508137035	0.540272037
H	3.030796218	0.799438056	0.788131057
N	-1.749006126	-0.432124030	0.219997017
H	-1.954863140	-1.392721101	0.418584030
H	-2.303200166	-0.089682007	-0.543891038
H	1.940422142	1.581051114	-1.255276090
O	2.351911170	-1.075651080	2.137841155
O	-2.870726207	0.425988029	-2.766074199
H	-2.402418175	-0.142367011	-3.361889241
H	-2.421135174	1.266280093	-2.786699200
O	-1.206202086	2.744934198	-2.293296164
H	-1.517070108	3.476532248	-1.777719130
H	-0.783142058	2.131773154	-1.688415119
O	4.861567352	1.111179082	1.378857102
H	5.230761375	1.974148142	1.508285110
H	5.176342374	0.552358038	2.083569149
O	-2.275856164	-3.683598263	0.681468048
H	-2.807469200	-4.447300318	0.502444035
H	-1.641552119	-3.922996283	1.349164099
O	5.450944392	-0.887440063	3.423129247
H	4.684658339	-1.309065095	3.791900272
H	6.107292438	-1.564321112	3.317193237
O	-0.178674015	-3.374133244	2.689807195
H	-0.030319004	-2.629336189	2.113399151
H	-0.616389046	-3.033691220	3.458318248

Coord_2

C	-0.401755029	-0.210544017	0.057643003
N	0.397666029	-1.045499073	0.938988065
C	1.534106112	-0.534299039	1.176916084
C	1.509398107	0.794905060	-0.673017050
N	0.078742003	0.728872053	-0.657150046
N	2.121850154	0.500430034	0.550537039
H	3.052938222	0.792028055	0.787578056
N	-1.739003125	-0.451149032	0.192413012
H	-1.953262141	-1.405600101	0.411504030
H	-2.274806166	-0.113597009	-0.586500041
H	1.934253142	1.625795115	-1.212961087
O	2.356521171	-1.085582080	2.142966152
O	-2.840912202	0.411249030	-2.770153198
H	-2.399733172	-0.147367011	-3.394900244
H	-2.402681170	1.257076092	-2.805358201
O	-1.196445084	2.745019199	-2.301558166
H	-1.517345111	3.476039251	-1.791150130
H	-0.779324055	2.134990154	-1.690634123
O	4.875431351	1.128059080	1.380146098
H	5.231763377	1.993378142	1.528458108
H	5.185549376	0.564428042	2.083529149
O	-2.365140172	-3.660749263	0.747317055
H	-2.927158209	-4.413002319	0.616889045
H	-1.689450121	-3.911792283	1.368979098
O	5.425487389	-0.873804065	3.417856244
H	4.628517332	-1.288100092	3.726052270
H	6.074165440	-1.560614114	3.331095242
O	-0.151197010	-3.428261245	2.632726189
H	-0.063164004	-2.612325189	2.148331157
H	-0.477360033	-3.274157236	3.508955251

Coord_3

C	-0.390220029	-0.223749016	0.081023006
N	0.393167028	-1.034479074	0.968840070
C	1.553583111	-0.542800039	1.200875087
C	1.500206108	0.836360059	-0.631288048
N	0.090146006	0.729198052	-0.640596048
N	2.138679155	0.491485033	0.555944040
H	3.073781223	0.783053056	0.781644058
N	-1.726284123	-0.471918032	0.167818013
H	-1.949454139	-1.419772103	0.406546031
H	-2.245094159	-0.138912012	-0.624317042
H	1.926212140	1.665296122	-1.173919083
O	2.363628170	-1.096456080	2.143979156
O	-2.815161204	0.396269028	-2.769263201

H	-2.405177172	-0.153867011	-3.421963247
H	-2.387672174	1.246798088	-2.820144202
O	-1.189052087	2.744110200	-2.309060169
H	-1.518869110	3.474704248	-1.803575132
H	-0.776942053	2.137289154	-1.692809121
O	4.888631350	1.139619084	1.374500100
H	5.234749376	2.005598146	1.541907111
H	5.191765372	0.569328044	2.076056150
O	-2.403469174	-3.658948261	0.770196054
H	-3.001287215	-4.392324316	0.706119050
H	-1.718552123	-3.902312279	1.385243102
O	5.389704387	-0.869280065	3.403465243
H	4.564359326	-1.272070091	3.647069264
H	6.027363432	-1.568301112	3.335651242
O	-0.152246009	-3.446185246	2.607465188
H	-0.079412005	-2.596210186	2.183280155
H	-0.378280028	-3.432061245	3.527501252

Coord_4

C	-0.378384027	-0.237123018	0.104552010
N	0.390548029	-1.023267072	0.996713069
C	1.574309116	-0.551954038	1.222463089
C	1.489702109	0.873740061	-0.590596042
N	0.101688007	0.729254055	-0.624605047
N	2.153956153	0.481882032	0.558144041
H	3.092811225	0.773536057	0.771953055
N	-1.711510123	-0.493349033	0.145809012
H	-1.944405142	-1.434134105	0.403204028
H	-2.214290159	-0.164326014	-0.658112048
H	1.916893138	1.700105121	-1.136783080
O	2.371881171	-1.107819082	2.142609153
O	-2.792129199	0.382385025	-2.765304198
H	-2.417055175	-0.160385009	-3.444508246
H	-2.374601173	1.236714087	-2.832367202
O	-1.182498084	2.743087200	-2.315879168
H	-1.520325109	3.473386253	-1.815108132
H	-0.774981055	2.139362153	-1.694811120
O	4.899998352	1.148684081	1.365100097
H	5.237262376	2.014176147	1.551971110
H	5.194408374	0.570511040	2.064457151
O	-2.411787173	-3.664678261	0.767173055
H	-3.049672220	-4.366628315	0.772763056
H	-1.734145125	-3.892065281	1.396741102
O	5.345199384	-0.869025065	3.383749241
H	4.495092321	-1.256855091	3.559190259
H	5.969427429	-1.581484114	3.334916241
O	-0.165465010	-3.448312247	2.603168189

H	-0.084463007	-2.580684184	2.218241161
H	-0.301340021	-3.546725256	3.535632256

Coord_5

C	-0.366192027	-0.250412019	0.128607010
N	0.389478027	-1.011864075	1.023243074
C	1.596156114	-0.561657043	1.242258091
C	1.478179105	0.907248067	-0.550550041
N	0.113496010	0.729162052	-0.608756046
N	2.167743157	0.471882032	0.557803039
H	3.110191226	0.764043056	0.758801053
N	-1.694956120	-0.514634035	0.126679011
H	-1.938608138	-1.447831102	0.401805031
H	-2.182547155	-0.188885014	-0.687739052
H	1.906695136	1.730315125	-1.101222078
O	2.381157172	-1.119449080	2.139498152
O	-2.771405199	0.370412025	-2.758847199
H	-2.434830175	-0.165953012	-3.462809248
H	-2.362891169	1.227591087	-2.842320205
O	-1.175975085	2.742386198	-2.321813166
H	-1.520864108	3.472562250	-1.825527130
H	-0.772861054	2.141517154	-1.696380120
O	4.909099354	1.156775084	1.353819096
H	5.237879375	2.020929147	1.560885111
H	5.193326376	0.569785041	2.050613149
O	-2.399803171	-3.672531262	0.748391052
H	-3.081464220	-4.328410314	0.818726058
H	-1.739825123	-3.879252280	1.403900103
O	5.293024380	-0.870582063	3.360580242
H	4.422802317	-1.240626088	3.464543251
H	5.902004427	-1.597015117	3.330884238
O	-0.185193013	-3.441377247	2.613226187
H	-0.081821005	-2.565493182	2.253210162
H	-0.237019019	-3.634730263	3.539219257

Coord_6

C	-0.352958024	-0.263320017	0.154045011
N	0.390702030	-1.000100073	1.049280077
C	1.620138114	-0.571316041	1.260441093
C	1.466005107	0.937362068	-0.511174036
N	0.125843007	0.729052052	-0.592432044
N	2.180793155	0.462409035	0.554930041
H	3.126863226	0.756076055	0.741202052
N	-1.676232120	-0.535103039	0.111651007
H	-1.931674138	-1.460144104	0.403743027
H	-2.149659154	-0.211896017	-0.711960050
H	1.895698139	1.756258124	-1.067667076

O	2.393045170	-1.130412082	2.134539152
O	-2.753191199	0.360746026	-2.749228196
H	-2.458745177	-0.169943014	-3.476019248
H	-2.352693172	1.219824088	-2.849264207
O	-1.169353083	2.742211200	-2.326137168
H	-1.520191111	3.472472252	-1.833992130
H	-0.770379054	2.143911157	-1.696851120
O	4.915889354	1.165875086	1.342621097
H	5.235273378	2.027968146	1.571690112
H	5.188508376	0.569020041	2.036269149
O	-2.373139173	-3.676753266	0.719278053
H	-3.101466221	-4.271702310	0.843039059
H	-1.738697123	-3.860620277	1.406723100
O	5.233991377	-0.872348065	3.334822238
H	4.349343312	-1.222694086	3.363746241
H	5.826623419	-1.612565117	3.324344237
O	-0.210451014	-3.427405248	2.633930189
H	-0.074151004	-2.550302186	2.288178162
H	-0.180645015	-3.703818269	3.539545257

Coord_7

C	-0.337496025	-0.273836018	0.185208015
N	0.397117029	-0.986356070	1.077644078
C	1.650064120	-0.577668041	1.276246093
C	1.451822104	0.966968069	-0.472733034
N	0.137435010	0.730743054	-0.572328039
N	2.194785157	0.458255036	0.547799039
H	3.145321224	0.756124056	0.713266049
N	-1.654577118	-0.552473039	0.107694010
H	-1.922216137	-1.468801105	0.416433030
H	-2.116541152	-0.230897015	-0.722915051
H	1.880458136	1.780720126	-1.038042077
O	2.414476171	-1.136671080	2.124676151
O	-2.743057195	0.356218025	-2.728852194
H	-2.495676182	-0.168917013	-3.476982250
H	-2.349677168	1.216254089	-2.845819205
O	-1.167052082	2.744877200	-2.322831165
H	-1.521616111	3.475342251	-1.833486130
H	-0.770762057	2.148601154	-1.691138122
O	4.919697356	1.178744084	1.337879097
H	5.226253377	2.036983146	1.596671114
H	5.177346371	0.568157043	2.025863148
O	-2.336232166	-3.646312260	0.666387046
H	-3.116591223	-4.163036301	0.820112058
H	-1.738773124	-3.815368272	1.390731099
O	5.163631372	-0.879591062	3.304386238
H	4.271713306	-1.209451086	3.251067233

H	5.739961415	-1.632486116	3.311724238
O	-0.251395019	-3.405877243	2.658900190
H	-0.066107002	-2.534156184	2.323127166
H	-0.144146009	-3.761940272	3.530105254

Coord_8

C	-0.326166023	-0.275218017	0.220049014
N	0.385966026	-0.971209070	1.114780081
C	1.662252120	-0.592327045	1.317172095
C	1.445454106	0.995916070	-0.406647030
N	0.158014009	0.742776052	-0.540074040
N	2.200601159	0.443414032	0.572029044
H	3.151978226	0.745227053	0.726612053
N	-1.636711120	-0.551738038	0.092199007
H	-1.926812137	-1.458447106	0.409490029
H	-2.075752148	-0.224849017	-0.748586054
H	1.884318135	1.804777132	-0.971763071
O	2.403692174	-1.157892082	2.148238154
O	-2.704874194	0.384400026	-2.725691196
H	-2.501771182	-0.133200010	-3.492306250
H	-2.312986166	1.243562090	-2.852092204
O	-1.129121080	2.770907201	-2.311883165
H	-1.488763105	3.501284250	-1.825946132
H	-0.744501054	2.172296156	-1.676424121
O	4.925531355	1.234258090	1.291216094
H	5.211878373	2.100985150	1.544420110
H	5.207021377	0.633541046	1.979223143
O	-2.326671166	-3.649657263	0.642695045
H	-3.146205225	-4.092832292	0.819438061
H	-1.760317125	-3.791929271	1.398000099
O	5.210315374	-0.785453055	3.276399233
H	4.319932313	-1.112325079	3.183406227
H	5.784278417	-1.539702109	3.299659235
O	-0.317335023	-3.378236241	2.699407195
H	-0.090461004	-2.518680184	2.358090171
H	-0.109238007	-3.802298272	3.520400254

Coord_9

C	-0.339245025	-0.293003019	0.227426014
N	0.352357026	-0.969183067	1.123298083
C	1.646772119	-0.631536047	1.335461096
C	1.425364104	0.999111073	-0.361346028
N	0.162160013	0.738264054	-0.534950038
N	2.183601160	0.395304031	0.576986043
H	3.134961225	0.683721052	0.737851053
N	-1.641860116	-0.567363039	0.052061003
H	-1.954944141	-1.463450107	0.378266026

H	-2.059006149	-0.236089016	-0.797965059
H	1.883311137	1.800017130	-0.923271067
O	2.356706172	-1.207918086	2.153177156
O	-2.682929192	0.391810027	-2.742325195
H	-2.526368182	-0.120827010	-3.523260256
H	-2.291903163	1.249353088	-2.881434209
O	-1.106463081	2.777712198	-2.330536166
H	-1.471501105	3.509378254	-1.850499131
H	-0.734238053	2.178362157	-1.689901123
O	4.913904352	1.200204084	1.239440090
H	5.207279372	2.066886148	1.484749105
H	5.190653375	0.600349044	1.931167139
O	-2.248145163	-3.703743269	0.631082044
H	-3.089309220	-4.098997297	0.817436057
H	-1.709593121	-3.806792272	1.412419100
O	5.135911370	-0.790154059	3.245908236
H	4.239800304	-1.081674080	3.095754223
H	5.677697409	-1.566404112	3.295356236
O	-0.330558025	-3.352313239	2.751657199
H	-0.063679005	-2.509808183	2.393189170
H	0.013590002	-3.835015274	3.490543253

Coord_10

C	-0.357476028	-0.325875023	0.229680018
N	0.341885027	-0.973917071	1.110492078
C	1.653274120	-0.646333049	1.306678092
C	1.358668096	1.022653073	-0.350634025
N	0.124605007	0.729787053	-0.539943037
N	2.151526155	0.392262029	0.530966037
H	3.102758223	0.691790052	0.672735046
N	-1.649147119	-0.620508046	0.029419001
H	-1.963775141	-1.512845109	0.364878027
H	-2.065503149	-0.287993023	-0.820383060
H	1.807123128	1.824952131	-0.918745067
O	2.363013171	-1.219113085	2.093251151
O	-2.733839197	0.356619025	-2.728166195
H	-2.629401188	-0.143525009	-3.525973252
H	-2.360519169	1.219526087	-2.880668210
O	-1.191319087	2.765921198	-2.329191167
H	-1.566105111	3.489871251	-1.844840131
H	-0.810044059	2.169065158	-1.692877120
O	4.862872351	1.248671090	1.181207087
H	5.136525369	2.113660152	1.453307107
H	5.132414370	0.636409044	1.865785136
O	-2.145668152	-3.642177264	0.683196049
H	-2.886480206	-4.220391304	0.804450057
H	-1.559679111	-3.776041274	1.425256104

O	5.025804364	-0.758670055	3.159791227
H	4.140683299	-1.031827075	2.927287212
H	5.552154399	-1.544063112	3.226183233
O	-0.264665017	-3.327435241	2.832781203
H	-0.002365999	-2.522987184	2.391665171
H	0.533658036	-3.727547270	3.149010225

Relaxation pathway III'

LIIC path connecting T1-MIN and S₁/T₁/S₀-II

Coord_1

C	-0.423898028	-0.152036010	0.053306003
N	0.319811022	-0.996880072	0.905004064
C	1.620508115	-0.606153044	1.180635083
C	1.489371108	0.936257066	-0.624707046
N	0.107005006	0.759349053	-0.687253050
N	2.169131157	0.388648029	0.461328031
H	3.110036225	0.672011047	0.668896050
N	-1.759399125	-0.405889031	0.087894007
H	-1.987531141	-1.344138095	0.363768025
H	-2.262516162	-0.086644006	-0.720380054
H	1.870221133	1.872892134	-0.993036070
O	2.195130159	-1.198825086	2.086624153
O	-2.870002208	0.416966028	-2.755116198
H	-2.577399183	-0.113193009	-3.483789253
H	-2.472259178	1.276549089	-2.859336207
O	-1.273743090	2.788246202	-2.379464170
H	-1.571062111	3.520601251	-1.856362135
H	-0.814580060	2.190624157	-1.794270127
O	4.907009353	1.193007083	1.250597089
H	5.165241373	2.066870151	1.510222110
H	5.169779370	0.597335041	1.948988140
O	-1.908706136	-3.461944250	0.868896062
H	-2.353677172	-4.294625310	0.785986058
H	-1.276836094	-3.549353256	1.577374116
O	5.005178363	-0.855862061	3.243423235
H	4.115876295	-1.110795080	3.020890216
H	5.519218396	-1.651977117	3.290351235
O	0.129721008	-3.457999249	3.051432221
H	0.705336053	-2.771724198	2.735364196
H	-0.116294008	-3.217004231	3.935135281

Coord_2

C	-0.439740034	-0.147772011	0.062571003
N	0.316009021	-0.978188071	0.898771065
C	1.613460115	-0.579732044	1.179117085
C	1.484093105	0.940366069	-0.634540048

N	0.087336006	0.802417059	-0.646372044
N	2.160814158	0.432466032	0.474108032
H	3.108632223	0.696254048	0.676480049
N	-1.771167127	-0.417358032	0.088061005
H	-1.992823141	-1.355929095	0.369146027
H	-2.268371164	-0.109712007	-0.726590050
H	1.885271135	1.833215133	-1.080551076
O	2.196195160	-1.175256087	2.075383147
O	-2.817994202	0.401771026	-2.768317201
H	-2.530545184	-0.124290009	-3.502156254
H	-2.436116177	1.267032091	-2.873914209
O	-1.292174095	2.826753202	-2.401336171
H	-1.656794117	3.566956258	-1.937487139
H	-0.826833059	2.289765165	-1.761381126
O	4.921615354	1.181684087	1.256123091
H	5.184510373	2.050665146	1.527278112
H	5.172773370	0.576744039	1.950783141
O	-1.897429136	-3.467562250	0.883014061
H	-2.364113171	-4.290570310	0.826381057
H	-1.263148088	-3.552043254	1.589875113
O	4.986980360	-0.884017064	3.234467233
H	4.094718296	-1.122940079	3.005690219
H	5.489661397	-1.687885122	3.270155238
O	0.144691009	-3.457766247	3.062373220
H	0.709124052	-2.742625196	2.792988201
H	-0.067959006	-3.368133242	3.982289287

Coord_3

C	-0.455076035	-0.147976009	0.071686007
N	0.311453022	-0.963556072	0.894229063
C	1.605771116	-0.556868041	1.179739086
C	1.476449108	0.936307068	-0.642898048
N	0.068693007	0.838952059	-0.603886043
N	2.150429155	0.472368034	0.487745036
H	3.104483224	0.718801053	0.683128050
N	-1.782661127	-0.430802029	0.086621008
H	-1.999386145	-1.369219096	0.372964025
H	-2.273226164	-0.133433012	-0.734459053
H	1.893634136	1.778453130	-1.165226082
O	2.196272161	-1.154135083	2.067074149
O	-2.767611200	0.392914028	-2.779250199
H	-2.487927180	-0.127040011	-3.520554255
H	-2.398485171	1.262765091	-2.883930206
O	-1.301681093	2.860812204	-2.413670176
H	-1.718519124	3.606978261	-2.008934143
H	-0.838599061	2.381201173	-1.726077124
O	4.932379354	1.173410083	1.257861089

H	5.198404377	2.038614145	1.537965111
H	5.173364371	0.561798042	1.950254139
O	-1.890076134	-3.474522248	0.896023064
H	-2.378016171	-4.286660309	0.867704064
H	-1.253673090	-3.554072257	1.601734113
O	4.969771357	-0.902976067	3.227326230
H	4.075088291	-1.128052079	2.993615214
H	5.462489394	-1.713302124	3.253659233
O	0.154887011	-3.452677250	3.072916219
H	0.707699052	-2.714745196	2.843120205
H	-0.005652999	-3.509028251	4.005931286

Coord_4

C	-0.469722031	-0.152944010	0.080620006
N	0.306298021	-0.953362070	0.891395065
C	1.597615114	-0.538016038	1.182582085
C	1.466707108	0.923293065	-0.649501048
N	0.051405003	0.868670061	-0.559737039
N	2.138119153	0.507925036	0.502247038
H	3.097787222	0.739305052	0.688946047
N	-1.793795127	-0.446487033	0.083421004
H	-2.007193145	-1.384301098	0.374991027
H	-2.277020164	-0.157963013	-0.744143055
H	1.895593134	1.707623121	-1.246137088
O	2.195457159	-1.136003084	2.061813148
O	-2.719244198	0.389539025	-2.788252203
H	-2.449835176	-0.122230007	-3.539131255
H	-2.360045169	1.263169091	-2.889890208
O	-1.303288093	2.891415207	-2.416842176
H	-1.758250127	3.643724260	-2.069920149
H	-0.849710064	2.464725176	-1.688126119
O	4.939641354	1.168116083	1.256040090
H	5.207210373	2.030772145	1.542524111
H	5.172041375	0.552381042	1.947689142
O	-1.886694135	-3.483206253	0.907559064
H	-2.395293173	-4.283134311	0.909339063
H	-1.248491090	-3.555748257	1.612589115
O	4.954308358	-0.913043066	3.222365230
H	4.057670290	-1.126600080	2.984972215
H	5.438581393	-1.728605126	3.241270235
O	0.160110012	-3.442869246	3.082740220
H	0.701314052	-2.687310192	2.883865207
H	0.069398003	-3.634524260	4.007116289

Coord_5

C	-0.483561032	-0.162865014	0.089442004
N	0.300646021	-0.947901067	0.890339065

C	1.589123115	-0.523555037	1.187761085
C	1.455003104	0.900618063	-0.653917048
N	0.035734001	0.891406066	-0.513717039
N	2.123940155	0.538799041	0.517652038
H	3.088649225	0.757509056	0.694007051
N	-1.804494128	-0.464603035	0.078428005
H	-2.016228143	-1.401398100	0.375089026
H	-2.279645163	-0.183394012	-0.755696053
H	1.891271138	1.619833118	-1.322115098
O	2.193830156	-1.121363083	2.059700149
O	-2.672795194	0.390867028	-2.795598199
H	-2.415928176	-0.110565009	-3.557872258
H	-2.321005165	1.267684090	-2.892188208
O	-1.297840092	2.919333212	-2.411137174
H	-1.778043129	3.679293264	-2.119983153
H	-0.859898064	2.540399184	-1.647093118
O	4.943647358	1.165811082	1.250716090
H	5.211109378	2.027239146	1.541031111
H	5.169247372	0.548448038	1.943142139
O	-1.887412134	-3.493929252	0.917297063
H	-2.415972171	-4.280172310	0.950674066
H	-1.247772092	-3.557339255	1.622094118
O	4.941400355	-0.914448068	3.219635231
H	4.043202293	-1.118979081	2.979821214
H	5.418886390	-1.734068124	3.233007233
O	0.160068011	-3.428481245	3.091508221
H	0.690110052	-2.659746191	2.913183209
H	0.155406012	-3.740122268	3.987195289

Coord_6

C	-0.496516038	-0.177868015	0.098273009
N	0.294535019	-0.947414070	0.891194062
C	1.580374111	-0.513820038	1.195446088
C	1.441363106	0.867575061	-0.655565049
N	0.021908002	0.907026066	-0.465537033
N	2.107857152	0.564684042	0.534041039
H	3.077068223	0.773197055	0.698362052
N	-1.814699131	-0.485273037	0.071668004
H	-2.026489143	-1.420661104	0.373175029
H	-2.280970165	-0.209764015	-0.769111056
H	1.880657133	1.514190109	-1.391761100
O	2.191424156	-1.110684079	2.060882151
O	-2.627915190	0.396234028	-2.801474204
H	-2.385572171	-0.092621005	-3.576642260
H	-2.281286163	1.275808093	-2.891089207
O	-1.285956093	2.945085210	-2.396745172
H	-1.779562127	3.714988269	-2.158742153

H	-0.868801064	2.608355190	-1.602483116
O	4.944524358	1.166582083	1.241793088
H	5.210144375	2.028164148	1.533394110
H	5.165340372	0.550056038	1.936483137
O	-1.892394136	-3.506935254	0.924979066
H	-2.440137177	-4.277888307	0.991161074
H	-1.251719087	-3.559016255	1.629955120
O	4.931853357	-0.907279066	3.218987232
H	4.032420291	-1.105451077	2.978079216
H	5.404367391	-1.729783127	3.228658232
O	0.154434009	-3.409529243	3.098878221
H	0.674198047	-2.631750190	2.928658209
H	0.250224018	-3.821899277	3.947488284

Coord_7

C	-0.508536034	-0.198062017	0.107276008
N	0.287946021	-0.952106068	0.894198064
C	1.571394111	-0.509126035	1.205914087
C	1.425753102	0.823366059	-0.653704049
N	0.010169998	0.915359068	-0.414875032
N	2.089766148	0.585250040	0.551549037
H	3.062951219	0.786151055	0.702065050
N	-1.824350134	-0.508545036	0.063207005
H	-2.037975147	-1.442147103	0.369238024
H	-2.280865166	-0.237037016	-0.784337057
H	1.863678132	1.389695102	-1.453414107
O	2.188196159	-1.104398078	2.065626151
O	-2.584209187	0.405097027	-2.805966205
H	-2.358134172	-0.068853003	-3.595214259
H	-2.240696162	1.287090094	-2.886753208
O	-1.268025092	2.968924211	-2.373814170
H	-1.763847129	3.751540272	-2.185761155
H	-0.875968061	2.668610190	-1.553884112
O	4.942265358	1.170553082	1.229069089
H	5.204193375	2.033723145	1.519365108
H	5.160565372	0.557360039	1.927475138
O	-1.901811136	-3.522343255	0.930485065
H	-2.467893175	-4.276292308	1.030416072
H	-1.260541091	-3.560783257	1.635990116
O	4.926414357	-0.891420063	3.220191232
H	4.026022289	-1.086094081	2.979633214
H	5.395944386	-1.715606125	3.227941234
O	0.142881011	-3.385769243	3.104550223
H	0.653770048	-2.603499190	2.927100211
H	0.351618025	-3.876327279	3.888840279

Coord_8

C	-0.519568036	-0.223545018	0.116673010
N	0.280783020	-0.962141068	0.899770067
C	1.562145114	-0.509780035	1.219636087
C	1.408122101	0.767014053	-0.647358044
N	0.000816002	0.916145066	-0.361410027
N	2.069510148	0.600092043	0.570409042
H	3.046125219	0.796083056	0.705232048
N	-1.833390132	-0.534357037	0.053158003
H	-2.050701146	-1.465758103	0.363384027
H	-2.279240163	-0.265073017	-0.801268056
H	1.840279131	1.245124089	-1.505059108
O	2.183990158	-1.102896077	2.074456151
O	-2.541442182	0.417002028	-2.809068205
H	-2.333263170	-0.039653003	-3.613289261
H	-2.199097158	1.301104094	-2.879287205
O	-1.244232092	2.990817216	-2.342561169
H	-1.731164126	3.789286274	-2.200498160
H	-0.880873063	2.720899194	-1.501135110
O	4.936726354	1.177831084	1.212308088
H	5.192971372	2.044061146	1.498581110
H	5.155023373	0.570584040	1.915873138
O	-1.915831137	-3.540065253	0.933976069
H	-2.499341179	-4.275196308	1.068397076
H	-1.274436090	-3.562342255	1.640258116
O	4.925701354	-0.866495063	3.223109232
H	4.024595288	-1.060747078	2.984509217
H	5.394417387	-1.691102122	3.230727231
O	0.125107011	-3.356476240	3.108366226
H	0.629264045	-2.576249186	2.903707211
H	0.457679031	-3.899859278	3.810809273

Coord_9

C	-0.529542037	-0.254390019	0.126846009
N	0.272835021	-0.977579073	0.908744067
C	1.552487111	-0.516047039	1.237500090
C	1.388496103	0.697212050	-0.635180046
N	-0.005721999	0.908987065	-0.304846022
N	2.046920148	0.608655041	0.591065042
H	3.026375218	0.802527059	0.708177052
N	-1.841779131	-0.562413041	0.041762002
H	-2.064724147	-1.491070106	0.356032025
H	-2.276141163	-0.293514019	-0.819661062
H	1.810582132	1.078764076	-1.544133111
O	2.178428156	-1.106433082	2.088467150
O	-2.499930180	0.431531029	-2.810673205
H	-2.311455167	-0.005452002	-3.630499264
H	-2.156721157	1.317368097	-2.868863207

O	-1.214606088	3.010340216	-2.303562165
H	-1.680633123	3.828339274	-2.202368161
H	-0.882928065	2.764339201	-1.444701103
O	4.927639354	1.188349085	1.191418086
H	5.176057375	2.059161150	1.470648108
H	5.148627372	0.589957045	1.901682139
O	-1.934599139	-3.559562254	0.936294066
H	-2.534552183	-4.273956308	1.105896078
H	-1.293559095	-3.562773254	1.643439117
O	4.930027357	-0.831758059	3.228082234
H	4.028457287	-1.028884072	2.993236217
H	5.400249386	-1.655444117	3.237542235
O	0.100892008	-3.319949240	3.110590226
H	0.601719041	-2.554192184	2.849865204
H	0.567778041	-3.887802282	3.709607267

Coord_10

C	-0.542679037	-0.313289024	0.155888013
N	0.271979019	-1.056551078	0.892797062
C	1.549357112	-0.594863042	1.246452091
C	1.348649098	0.646652048	-0.561765042
N	-0.026274000	0.894693067	-0.165181011
N	2.014081144	0.581812044	0.660302048
H	2.994884218	0.779150056	0.760245056
N	-1.852298133	-0.619415046	0.041062001
H	-2.072390147	-1.562821112	0.309467020
H	-2.284787163	-0.304507020	-0.807365057
H	1.746071124	0.978772071	-1.500164107
O	2.190152157	-1.222662086	2.055813146
O	-2.498641178	0.572666041	-2.731083195
H	-2.336800169	0.206473014	-3.590335261
H	-2.159778155	1.463796104	-2.729688199
O	-1.232392090	3.126873227	-2.046259147
H	-1.667943119	3.960723288	-1.927594139
H	-0.925171067	2.850878203	-1.191430088
O	4.906577354	1.166705085	1.221135087
H	5.139989368	2.029385145	1.536289112
H	5.143999373	0.543479037	1.904202139
O	-1.927764137	-3.653831265	0.783632055
H	-2.535338181	-4.361271316	0.955511069
H	-1.281447091	-3.668203264	1.486016109
O	4.965363358	-0.932913068	3.176402228
H	4.063382293	-1.131146083	2.943686214
H	5.446320394	-1.749595126	3.140434225
O	0.117196007	-3.450725248	2.952999215
H	0.611185043	-2.708221192	2.620999187
H	0.741587055	-4.028244288	3.372324241

LIIC path connecting S1-MIN and T1-MIN

Coord_1

C	-0.528514036	-0.198852015	0.053044002
N	0.272746019	-0.910152065	0.884654066
C	1.562816111	-0.642046047	1.248051090
C	1.456630102	0.873824062	-0.582809040
N	0.070876006	0.748146053	-0.594151045
N	2.110098154	0.394877027	0.566599039
H	3.079049219	0.607218045	0.725546052
N	-1.853804134	-0.459780034	0.017630000
H	-2.085728150	-1.385158100	0.332370023
H	-2.292495164	-0.199327015	-0.848195061
H	1.847113132	1.792133130	-0.988200073
O	2.132379151	-1.281374091	2.107923151
O	-2.789862203	0.433758029	-2.797952202
H	-2.500767179	-0.039636000	-3.565975258
H	-2.439824174	1.317267093	-2.865880208
O	-1.341935098	2.902234209	-2.304437165
H	-1.692337122	3.660765265	-1.855336134
H	-0.901531063	2.370124170	-1.651441118
O	4.913998355	1.132336081	1.249375092
H	5.124980367	2.000144144	1.565857113
H	5.128620371	0.515414037	1.946282139
O	-1.803395127	-3.468521251	0.881142065
H	-2.442738174	-4.155033300	1.014047074
H	-1.175779083	-3.528008256	1.597332115
O	4.875443353	-0.958641068	3.189077229
H	3.977989288	-1.155925083	2.933095212
H	5.358459386	-1.774142130	3.157625225
O	0.244686019	-3.374689245	3.029956218
H	0.891092063	-2.702802195	2.833502202
H	0.717654050	-4.099522294	3.415423246

Coord_2

C	-0.516689036	-0.197945015	0.058934005
N	0.284317019	-0.923457068	0.889765067
C	1.579258114	-0.639512044	1.242646090
C	1.460093107	0.882922064	-0.582646043
N	0.074075004	0.749060053	-0.597082041
N	2.121782155	0.394584027	0.556344039
H	3.088089223	0.616733043	0.717617050
N	-1.846438135	-0.460919035	0.029950004
H	-2.080757149	-1.391540099	0.332251021
H	-2.293936167	-0.192553011	-0.829199058
H	1.846750133	1.805036133	-0.982734069
O	2.148553152	-1.276847090	2.107837154

O	-2.803706200	0.435875029	-2.786106198
H	-2.514503181	-0.040233002	-3.552389257
H	-2.449398176	1.317160094	-2.854863204
O	-1.340866097	2.892990208	-2.298463167
H	-1.685597123	3.646692262	-1.837115133
H	-0.894456064	2.352184167	-1.656186118
O	4.919686355	1.141114084	1.245565089
H	5.135981369	2.009264144	1.557516110
H	5.141700368	0.524931036	1.940737140
O	-1.822214131	-3.485777250	0.856935063
H	-2.436228177	-4.201375304	0.951788069
H	-1.197098084	-3.548998257	1.571142112
O	4.902445352	-0.950304071	3.186358232
H	4.005354287	-1.154405085	2.935477214
H	5.389671387	-1.763562125	3.160666227
O	0.219855017	-3.375324242	3.003508215
H	0.848670061	-2.691691193	2.810650201
H	0.631532046	-4.059473292	3.515255254

Coord_3

C	-0.504647037	-0.197673013	0.063775003
N	0.295523019	-0.938078066	0.893395064
C	1.594303115	-0.638206045	1.235981092
C	1.463102104	0.891834065	-0.582490042
N	0.077095008	0.749483057	-0.600502045
N	2.132322154	0.393843030	0.546140042
H	3.095740221	0.625822044	0.710543051
N	-1.838024132	-0.462701035	0.041669004
H	-2.074125150	-1.397868101	0.332759026
H	-2.294131163	-0.186101013	-0.810505057
H	1.845851135	1.818004129	-0.976623072
O	2.163823155	-1.273827092	2.105491153
O	-2.816329204	0.437435033	-2.774560202
H	-2.526768182	-0.041382005	-3.538998257
H	-2.457924180	1.316659095	-2.844030205
O	-1.339403096	2.883624210	-2.292145166
H	-1.678664123	3.632261260	-1.818771129
H	-0.887778064	2.334014167	-1.660531119
O	4.923551354	1.150301082	1.243228089
H	5.144546373	2.018719144	1.551131110
H	5.153140370	0.534639041	1.936330141
O	-1.840545132	-3.501730251	0.836070060
H	-2.430257174	-4.241311306	0.896323065
H	-1.216578088	-3.569055255	1.547910114
O	4.928349357	-0.942543067	3.183805227
H	4.031869290	-1.153781084	2.937688212
H	5.420245391	-1.753199125	3.163498230

O	0.198397012	-3.379544245	2.979675214
H	0.812400057	-2.688058195	2.783767198
H	0.540840040	-4.006957287	3.604136262

Coord_4

C	-0.492578038	-0.197692016	0.067554006
N	0.306005021	-0.953651069	0.895640066
C	1.607622115	-0.637927047	1.228163090
C	1.465586104	0.900540063	-0.582472044
N	0.079837003	0.749623056	-0.604533042
N	2.141588153	0.392651027	0.535900038
H	3.101901226	0.634322043	0.704230051
N	-1.828744131	-0.464660033	0.052715002
H	-2.065905149	-1.403728099	0.333756023
H	-2.293264164	-0.179539014	-0.792181056
H	1.844497134	1.830898131	-0.970091072
O	2.178007158	-1.271875089	2.101104152
O	-2.828074204	0.438631032	-2.763402198
H	-2.537965181	-0.042962001	-3.525872254
H	-2.465674176	1.315926095	-2.833561205
O	-1.337632099	2.874251205	-2.285826165
H	-1.671559120	3.617653258	-1.800688132
H	-0.881545065	2.315771168	-1.664768119
O	4.925581352	1.159416081	1.242260092
H	5.150831369	2.028038146	1.546495110
H	5.162782371	0.544115039	1.933051137
O	-1.857676135	-3.515933252	0.818351057
H	-2.424236174	-4.275365306	0.847233059
H	-1.233751091	-3.587707261	1.527647113
O	4.952654357	-0.935551070	3.181603230
H	4.057006294	-1.154104083	2.939903210
H	5.449507390	-1.743354126	3.166435227
O	0.180513012	-3.387882243	2.959045213
H	0.782591058	-2.691761192	2.755139201
H	0.448021033	-3.943513284	3.681330263

Coord_5

C	-0.480650034	-0.197683014	0.070248005
N	0.315431022	-0.969840067	0.896575064
C	1.618920118	-0.638509047	1.219274087
C	1.467483104	0.909031066	-0.582707041
N	0.082213004	0.749682054	-0.609291044
N	2.149462157	0.390992030	0.525544040
H	3.106487224	0.642064044	0.698587048
N	-1.818763133	-0.466370032	0.063009003
H	-2.056128150	-1.408745102	0.335103022
H	-2.291504163	-0.172471010	-0.774301057

H	1.842775133	1.843607132	-0.963334071
O	2.190891158	-1.270627093	2.094872153
O	-2.839276203	0.439644030	-2.752705197
H	-2.548492183	-0.044846004	-3.513069255
H	-2.472929180	1.315114093	-2.823603201
O	-1.335673095	2.864983205	-2.279796164
H	-1.664351122	3.603033260	-1.783184128
H	-0.875833063	2.297601163	-1.669148119
O	4.925770353	1.168007083	1.242554092
H	5.154987373	2.036768147	1.543411112
H	5.170491372	0.552951040	1.930873138
O	-1.872821135	-3.527994254	0.803581058
H	-2.417295173	-4.304019312	0.804023059
H	-1.248068087	-3.604522259	1.510359109
O	4.974926358	-0.929550067	3.179896226
H	4.080296295	-1.155458084	2.942258213
H	5.476865393	-1.734342127	3.169732229
O	0.166435013	-3.400849244	2.942203210
H	0.759332056	-2.702658195	2.726764198
H	0.354948026	-3.870363277	3.746430272

Coord_6

C	-0.469027036	-0.197326016	0.071809003
N	0.323450026	-0.986320070	0.896249065
C	1.627882115	-0.639819046	1.209372086
C	1.468743107	0.917305065	-0.583319040
N	0.084140008	0.749868054	-0.614905043
N	2.155817153	0.388830029	0.514987038
H	3.109407224	0.648860045	0.693530050
N	-1.808219128	-0.467411035	0.072461003
H	-2.044774149	-1.412529100	0.336677023
H	-2.289013167	-0.164508014	-0.756939053
H	1.840784130	1.856032134	-0.956539070
O	2.202177160	-1.269778092	2.086974151
O	-2.850302204	0.440655034	-2.742521197
H	-2.558778182	-0.046903001	-3.500639251
H	-2.480003179	1.314378092	-2.814285204
O	-1.333684098	2.855933205	-2.274331165
H	-1.657146120	3.588563258	-1.766556125
H	-0.870748061	2.279647164	-1.673912122
O	4.924100354	1.175609085	1.244018087
H	5.157144374	2.044439148	1.541713110
H	5.176122374	0.560712038	1.929782139
O	-1.885056136	-3.537509253	0.791632056
H	-2.408249173	-4.327648310	0.766245053
H	-1.258801093	-3.619040258	1.496100110
O	4.994720360	-0.924804067	3.178826230

H	4.101258297	-1.157979084	2.944891214
H	5.501726395	-1.726524126	3.173631228
O	0.156536012	-3.419096244	2.929795210
H	0.742639054	-2.720691196	2.700427195
H	0.263078019	-3.788316271	3.798988273

Coord_7

C	-0.457879034	-0.196266015	0.072136003
N	0.329647025	-1.002749071	0.894663062
C	1.634114120	-0.641752046	1.198486084
C	1.469315105	0.925353067	-0.584460042
N	0.085533004	0.750408053	-0.621559045
N	2.160477156	0.386100030	0.504139037
H	3.110525222	0.654475050	0.688987048
N	-1.797234128	-0.467315032	0.080959007
H	-2.031731147	-1.414611100	0.338398024
H	-2.285951162	-0.155227013	-0.740182052
H	1.838655134	1.868070134	-0.949913067
O	2.211419161	-1.269072090	2.077567152
O	-2.861578204	0.441856034	-2.732897198
H	-2.569334184	-0.048992002	-3.488622250
H	-2.487268180	1.313885095	-2.805744204
O	-1.331864098	2.847219207	-2.269746162
H	-1.650084117	3.574415260	-1.751137128
H	-0.866429064	2.262061164	-1.679344121
O	4.920502357	1.181695084	1.246612088
H	5.157391373	2.050508150	1.541289112
H	5.179461371	0.566890039	1.929817139
O	-1.893222135	-3.543966253	0.782545056
H	-2.395533171	-4.346428313	0.733649052
H	-1.264920091	-3.630698261	1.485076105
O	5.011480361	-0.921670068	3.178580231
H	4.119300299	-1.161877083	2.947964215
H	5.523375396	-1.720357126	3.178430231
O	0.151479009	-3.443611248	2.922604210
H	0.732596053	-2.746002199	2.677779192
H	0.173683011	-3.697715268	3.838085275

Coord_8

C	-0.447414030	-0.194050012	0.071018005
N	0.333450026	-1.018720075	0.891737067
C	1.637027119	-0.644227045	1.186587084
C	1.469133105	0.933166068	-0.586351041
N	0.086287007	0.751589055	-0.629551045
N	2.163164154	0.382700029	0.492886035
H	3.109611222	0.658592049	0.684901048
N	-1.785901131	-0.465497033	0.088342009

H	-2.016739143	-1.414344104	0.340263024
H	-2.282488163	-0.144111010	-0.724153051
H	1.836563132	1.879594138	-0.943731070
O	2.217881161	-1.268291093	2.066771148
O	-2.873656209	0.443480031	-2.723877198
H	-2.580829183	-0.050947005	-3.477063251
H	-2.495211178	1.313837093	-2.798151204
O	-1.330475098	2.838989204	-2.266472164
H	-1.643344119	3.560802254	-1.737381123
H	-0.863067064	2.245025160	-1.685842122
O	4.914810351	1.185586087	1.250394091
H	5.155735371	2.054270150	1.542136113
H	5.180135374	0.570811042	1.931129138
O	-1.895725138	-3.546603254	0.776707056
H	-2.377031171	-4.360213317	0.706411050
H	-1.264866089	-3.638690261	1.477829107
O	5.024367362	-0.920666065	3.179462227
H	4.133534299	-1.167487082	2.951721214
H	5.540783401	-1.716484125	3.184568232
O	0.152445011	-3.476021248	2.921716208
H	0.729518051	-2.779120201	2.660445192
H	0.088230008	-3.598342258	3.861709276

Coord_9

C	-0.437932031	-0.190005012	0.068024005
N	0.333963026	-1.033666072	0.887214062
C	1.635631117	-0.647177044	1.173541087
C	1.468093108	0.940735070	-0.589364044
N	0.086258008	0.753828057	-0.639414046
N	2.163379154	0.378472029	0.481058035
H	3.106228223	0.660741048	0.681244047
N	-1.774267127	-0.461106031	0.094343006
H	-1.999235145	-1.410715102	0.342421025
H	-2.278808164	-0.130442012	-0.709049052
H	1.834768131	1.890440139	-0.938410066
O	2.220281160	-1.267257091	2.054613147
O	-2.887327207	0.445849031	-2.715525193
H	-2.594238186	-0.052549005	-3.466029250
H	-2.504531180	1.314516097	-2.791776200
O	-1.329898094	2.831460202	-2.265204165
H	-1.637178119	3.548033255	-1.726015126
H	-0.860948063	2.228812159	-1.694056122
O	4.906639352	1.186277086	1.255624093
H	5.152033374	2.054667149	1.544472113
H	5.177424372	0.571449039	1.934111137
O	-1.890122135	-3.544118253	0.775213057
H	-2.349689170	-4.368241316	0.685573050

H	-1.256077090	-3.641699263	1.475610108
O	5.031911360	-0.922644066	3.182022228
H	4.142440299	-1.175392085	2.956568213
H	5.552207401	-1.715939125	3.192794229
O	0.161591009	-3.519120254	2.928841209
H	0.734233052	-2.821327204	2.650180190
H	0.009097001	-3.489253251	3.865538276

Coord_10

C	-0.423898028	-0.152036010	0.053306003
N	0.319811022	-0.996880072	0.905004064
C	1.620508115	-0.606153044	1.180635083
C	1.489371108	0.936257066	-0.624707046
N	0.107005006	0.759349053	-0.687253050
N	2.169131157	0.388648029	0.461328031
H	3.110036225	0.672011047	0.668896050
N	-1.759399125	-0.405889031	0.087894007
H	-1.987531141	-1.344138095	0.363768025
H	-2.262516162	-0.086644006	-0.720380054
H	1.870221133	1.872892134	-0.993036070
O	2.195130159	-1.198825086	2.086624153
O	-2.870002208	0.416966028	-2.755116198
H	-2.577399183	-0.113193009	-3.483789253
H	-2.472259178	1.276549089	-2.859336207
O	-1.273743090	2.788246202	-2.379464170
H	-1.571062111	3.520601251	-1.856362135
H	-0.814580060	2.190624157	-1.794270127
O	4.907009353	1.193007083	1.250597089
H	5.165241373	2.066870151	1.510222110
H	5.169779370	0.597335041	1.948988140
O	-1.908706136	-3.461944250	0.868896062
H	-2.353677172	-4.294625310	0.785986058
H	-1.276836094	-3.549353256	1.577374116
O	5.005178363	-0.855862061	3.243423235
H	4.115876295	-1.110795080	3.020890216
H	5.519218396	-1.651977117	3.290351235
O	0.129721008	-3.457999249	3.051432221
H	0.705336053	-2.771724198	2.735364196
H	-0.116294008	-3.217004231	3.935135281

LIIC path connecting S₂/S₁/T₂ and T2-MIN

Coord_1

C	-0.451273034	-0.206392013	0.003103000
N	0.335008024	-1.025556076	0.800971056
C	1.561200115	-0.634017047	1.249789088
C	1.504268109	0.801837060	-0.576528040
N	0.103719005	0.776500058	-0.629494047

N	2.086553148	0.474402033	0.654833049
H	3.051260222	0.693035047	0.829636058
N	-1.761930126	-0.481940035	-0.002097002
H	-2.016053144	-1.396358100	0.328027023
H	-2.290486164	-0.124101008	-0.777553057
H	1.994073142	1.580866114	-1.135219081
O	2.132567152	-1.260817089	2.127673152
O	-2.838203206	0.497246038	-2.731611197
H	-2.537536182	-0.004727003	-3.476592252
H	-2.441886177	1.360718096	-2.801908204
O	-1.257381088	2.873063207	-2.287704162
H	-1.536893109	3.643065260	-1.810262128
H	-0.797474057	2.310325167	-1.670300122
O	4.915076353	1.160494084	1.263647092
H	5.156067371	2.031405147	1.548772112
H	5.158310374	0.554636041	1.960138143
O	-1.928169138	-3.446720249	0.836115061
H	-2.584562185	-4.117765299	0.966918067
H	-1.286629091	-3.539599254	1.536491109
O	4.935176357	-0.916059064	3.232391234
H	4.031943290	-1.122353083	3.011176215
H	5.419615390	-1.731207127	3.208732232
O	0.132418007	-3.422491244	2.982061216
H	0.753433053	-2.739870199	2.750735197
H	0.630725045	-4.109244296	3.403984244

Coord_2

C	-0.459332033	-0.205205015	0.009320002
N	0.325690023	-1.012174073	0.814141060
C	1.561827110	-0.635481047	1.249271092
C	1.501312109	0.810966060	-0.579184044
N	0.102479006	0.772100055	-0.627127048
N	2.093928148	0.460926031	0.641397048
H	3.058822218	0.679155051	0.815843058
N	-1.771931127	-0.478208034	-0.000939999
H	-2.024845143	-1.393300101	0.328476024
H	-2.291583164	-0.132481011	-0.787987057
H	1.978827144	1.610493118	-1.119432083
O	2.132229151	-1.263074094	2.126139152
O	-2.831360204	0.495113035	-2.741040199
H	-2.531840182	-0.003403001	-3.488758254
H	-2.439454174	1.360272095	-2.810916203
O	-1.261779091	2.879189207	-2.291680167
H	-1.548054113	3.647981264	-1.816267131
H	-0.803657059	2.319096169	-1.671140122
O	4.918925355	1.152151081	1.263199090
H	5.157987369	2.022725148	1.550976114

H	5.157767369	0.545435040	1.960507144
O	-1.917881138	-3.447710250	0.841481061
H	-2.571050184	-4.122220299	0.970605072
H	-1.277535090	-3.537419256	1.543476111
O	4.928837353	-0.924398066	3.230425235
H	4.025903288	-1.128028081	3.004853214
H	5.411646388	-1.740460125	3.205769231
O	0.141646012	-3.416556246	2.987212217
H	0.766153055	-2.735130199	2.760447198
H	0.635976045	-4.106619297	3.408395243

Coord_3

C	-0.467195035	-0.203741014	0.015630001
N	0.316800025	-0.998420073	0.827058060
C	1.562509114	-0.636905047	1.248863091
C	1.498271108	0.819924057	-0.581333043
N	0.101280006	0.767885058	-0.624522046
N	2.100882151	0.447460031	0.628082043
H	3.065972223	0.665283050	0.802102056
N	-1.781708126	-0.474150033	0.000400000
H	-2.033364146	-1.389980101	0.328872024
H	-2.291918165	-0.140125008	-0.797942056
H	1.963664141	1.639139118	-1.102513080
O	2.131877153	-1.265339089	2.124757152
O	-2.823894201	0.492441034	-2.750246200
H	-2.525327184	-0.002819001	-3.500483250
H	-2.436562178	1.359420099	-2.819788203
O	-1.266210093	2.885336209	-2.295401167
H	-1.559403113	3.652960261	-1.822272129
H	-0.809934059	2.328062167	-1.671553119
O	4.922161354	1.143974080	1.262998093
H	5.159125370	2.014203145	1.553536109
H	5.156682370	0.536353041	1.961041142
O	-1.907338139	-3.448307246	0.846689060
H	-2.557319182	-4.126214296	0.974113068
H	-1.268257094	-3.534943257	1.550304112
O	4.922197354	-0.932793067	3.228438232
H	4.019626288	-1.133878082	2.998482216
H	5.403520390	-1.749675127	3.202695230
O	0.150935009	-3.410510248	2.992289218
H	0.778962055	-2.730395195	2.770097200
H	0.641170047	-4.103831295	3.412894244

Coord_4

C	-0.474861036	-0.202015013	0.022023002
N	0.308345021	-0.984309070	0.839704063
C	1.563258111	-0.638298048	1.248557089

C	1.495163107	0.828711062	-0.582997041
N	0.100126008	0.763844054	-0.621694043
N	2.107427153	0.434004033	0.614879044
H	3.072716222	0.651422046	0.788415055
N	-1.791264131	-0.469784035	0.001929999
H	-2.041616146	-1.386416097	0.329234023
H	-2.291520165	-0.147063009	-0.807411058
H	1.948616139	1.666803118	-1.084511079
O	2.131514153	-1.267619091	2.123525154
O	-2.815801202	0.489263034	-2.759229201
H	-2.517994179	-0.002936002	-3.511775252
H	-2.433199177	1.358190100	-2.828517204
O	-1.270661093	2.891507210	-2.298862166
H	-1.570915116	3.658003262	-1.828270131
H	-0.816304056	2.337214166	-1.671543123
O	4.924771356	1.135982080	1.263081089
H	5.159448369	2.005858142	1.556501111
H	5.155042371	0.527402039	1.961771142
O	-1.896556137	-3.448533247	0.851757059
H	-2.543386184	-4.129767298	0.977465072
H	-1.258808089	-3.532189254	1.556991113
O	4.915246356	-0.941249070	3.226443234
H	4.013109290	-1.139917080	2.992063217
H	5.395241390	-1.758851124	3.199523231
O	0.160287011	-3.404357245	2.997300214
H	0.791856057	-2.725668198	2.779686199
H	0.646315046	-4.100879295	3.417493245

Coord_5

C	-0.482324033	-0.200042013	0.028486003
N	0.300333024	-0.969857070	0.852063061
C	1.564081114	-0.639665045	1.248347091
C	1.492003109	0.837329062	-0.584197041
N	0.099025007	0.759966053	-0.618656047
N	2.113572150	0.420554030	0.601781045
H	3.079063221	0.637573044	0.774782058
N	-1.800602130	-0.465126032	0.003659001
H	-2.049605146	-1.382621097	0.329577025
H	-2.290410163	-0.153318011	-0.816387058
H	1.933717138	1.693481123	-1.065476075
O	2.131143152	-1.269925092	2.122437155
O	-2.807077202	0.485610033	-2.767982200
H	-2.509838182	-0.003720000	-3.522634255
H	-2.429356175	1.356601097	-2.837095204
O	-1.275119094	2.897704208	-2.302059164
H	-1.582565112	3.663107266	-1.834250130
H	-0.822768057	2.346540169	-1.671113119

O	4.926739356	1.128195084	1.263486090
H	5.158923372	1.997710146	1.559922115
H	5.152831373	0.518597038	1.962733144
O	-1.885549133	-3.448403250	0.856704062
H	-2.529269184	-4.132893296	0.980684068
H	-1.249200087	-3.529171256	1.563555112
O	4.907971355	-0.949773068	3.224454231
H	4.006343288	-1.146163080	2.985594215
H	5.386812385	-1.767985126	3.196266229
O	0.169700010	-3.398101243	3.002251218
H	0.804829059	-2.720952197	2.789210199
H	0.651413045	-4.097762293	3.422200244

Coord_6

C	-0.489576037	-0.197836016	0.035009002
N	0.292774023	-0.955075070	0.864119063
C	1.564991114	-0.641013045	1.248225089
C	1.488811106	0.845777060	-0.584951044
N	0.097983004	0.756239052	-0.615421044
N	2.119330154	0.407108028	0.588782044
H	3.085022223	0.623740043	0.761204052
N	-1.809722129	-0.460191036	0.005592001
H	-2.057333150	-1.378609098	0.329916022
H	-2.288604166	-0.158913013	-0.824862059
H	1.918999136	1.719170123	-1.045454077
O	2.130766156	-1.272265093	2.121491155
O	-2.797719199	0.481505036	-2.776495202
H	-2.500859182	-0.005143000	-3.533060253
H	-2.425025177	1.354672098	-2.845512203
O	-1.279574094	2.903926211	-2.304986165
H	-1.594330114	3.668267263	-1.840202130
H	-0.829328061	2.356030169	-1.670269118
O	4.928051356	1.120632083	1.264252090
H	5.157513369	1.989773143	1.563849112
H	5.150032369	0.509950038	1.963960142
O	-1.874334137	-3.447935251	0.861544060
H	-2.514988183	-4.135606298	0.983787068
H	-1.239447091	-3.525903253	1.570009111
O	4.900360352	-0.958371071	3.222484231
H	3.999325286	-1.152635082	2.979071217
H	5.378234385	-1.777076127	3.192937228
O	0.179172013	-3.391746242	3.007146218
H	0.817873056	-2.716248197	2.798667199
H	0.656464047	-4.094477293	3.427023245

Coord_7

C	-0.496607035	-0.195409013	0.041584002
---	--------------	--------------	-------------

N	0.285683021	-0.939976066	0.875854066
C	1.566000112	-0.642348048	1.248185088
C	1.485606107	0.854058059	-0.585278044
N	0.097009006	0.752656056	-0.612002045
N	2.124716152	0.393663031	0.575877041
H	3.090605223	0.609923045	0.747681055
N	-1.818621129	-0.454993033	0.007736000
H	-2.064804148	-1.374391100	0.330265025
H	-2.286115165	-0.163862011	-0.832827060
H	1.904493139	1.743869127	-1.024495076
O	2.130385153	-1.274648094	2.120687155
O	-2.787723200	0.476973035	-2.784756198
H	-2.491056179	-0.007178998	-3.543047257
H	-2.420198176	1.352418099	-2.853757207
O	-1.284019093	2.910171212	-2.307639164
H	-1.606193114	3.673477267	-1.846118131
H	-0.835987058	2.365670170	-1.669014121
O	4.928692353	1.113313080	1.265416089
H	5.155182370	1.982066142	1.568333112
H	5.146629373	0.501472037	1.965487141
O	-1.862927134	-3.447142247	0.866290060
H	-2.500562181	-4.137919300	0.986787069
H	-1.229566087	-3.522400253	1.576365112
O	4.892399351	-0.967052071	3.220548231
H	3.992046289	-1.159350082	2.972491215
H	5.369510385	-1.786125126	3.189548229
O	0.188694013	-3.385296243	3.011987216
H	0.830977062	-2.711558195	2.808054200
H	0.661464047	-4.091024295	3.431968248

Coord_8

C	-0.503406037	-0.192774012	0.048200004
N	0.279073021	-0.924572065	0.887253062
C	1.567124111	-0.643675045	1.248222088
C	1.482407109	0.862171061	-0.585194042
N	0.096114009	0.749205053	-0.608410043
N	2.129745156	0.380218029	0.563060040
H	3.095824223	0.596124045	0.734215055
N	-1.827293132	-0.449542032	0.010100999
H	-2.072017152	-1.369976100	0.330637026
H	-2.282949166	-0.168178012	-0.840270060
H	1.890233135	1.767577125	-1.002643072
O	2.130002151	-1.277086093	2.120026154
O	-2.777087198	0.472031033	-2.792752199
H	-2.480432178	-0.009808999	-3.552586254
H	-2.414871176	1.349849097	-2.861816207
O	-1.288447095	2.916436210	-2.310013164

H	-1.618135115	3.678731267	-1.851989136
H	-0.842748060	2.375448169	-1.667350118
O	4.928644357	1.106254077	1.267019089
H	5.151891369	1.974601145	1.573427115
H	5.142604372	0.493176035	1.967350141
O	-1.851347132	-3.446040246	0.870951064
H	-2.486015178	-4.139844299	0.989695073
H	-1.219572088	-3.518676253	1.582634116
O	4.884076351	-0.975826073	3.218658232
H	3.984503285	-1.166328083	2.965850215
H	5.360642385	-1.795130130	3.186112228
O	0.198259013	-3.378756242	3.016777218
H	0.844128059	-2.706885194	2.817367201
H	0.666406049	-4.087402294	3.437043248

Coord_9

C	-0.509957039	-0.189939013	0.054852005
N	0.272962018	-0.908873064	0.898297065
C	1.568379113	-0.645002047	1.248330088
C	1.479235104	0.870118065	-0.584717042
N	0.095311009	0.745881053	-0.604655044
N	2.134435153	0.366769026	0.550325040
H	3.100695225	0.582346042	0.720805052
N	-1.835732133	-0.443848031	0.012692999
H	-2.078971149	-1.365371099	0.331045021
H	-2.279110165	-0.171867012	-0.847180062
H	1.876249134	1.790295128	-0.979944072
O	2.129618153	-1.279590091	2.119507153
O	-2.765808197	0.466691031	-2.800463200
H	-2.468988175	-0.013018999	-3.561664258
H	-2.409039172	1.346974099	-2.869676208
O	-1.292856094	2.922714210	-2.312104166
H	-1.630144115	3.684020266	-1.857808133
H	-0.849616061	2.385350171	-1.665283120
O	4.927892354	1.099472078	1.269104089
H	5.147602371	1.967394142	1.579186114
H	5.137939373	0.485070034	1.969584142
O	-1.839611135	-3.444640249	0.875535062
H	-2.471371177	-4.141390301	0.992518069
H	-1.209488087	-3.514742254	1.588823114
O	4.875375348	-0.984701068	3.216828232
H	3.976688285	-1.173590083	2.959142211
H	5.351633386	-1.804093128	3.182642228
O	0.207854013	-3.372129244	3.021516217
H	0.857313060	-2.702231197	2.826603202
H	0.671282047	-4.083612294	3.442251247

Coord_10

C	-0.523438036	-0.197572014	0.062985005
N	0.271008021	-0.896583066	0.906102065
C	1.572471114	-0.637488047	1.239901088
C	1.455305106	0.887513063	-0.590476041
N	0.075146006	0.738650052	-0.601153044
N	2.128303153	0.368422027	0.527469038
H	3.093328221	0.593078042	0.693032052
N	-1.848773135	-0.461649036	0.022822002
H	-2.079924150	-1.386961102	0.338974023
H	-2.286014166	-0.202093014	-0.843988059
H	1.830797132	1.825770133	-0.963882071
O	2.142177154	-1.268604091	2.107309152
O	-2.780555198	0.430916030	-2.795451199
H	-2.482203181	-0.043150002	-3.559686256
H	-2.438437174	1.317243095	-2.865619208
O	-1.346122097	2.912755211	-2.305690167
H	-1.696506123	3.669207262	-1.853003134
H	-0.897228064	2.382873172	-1.657166118
O	4.911818351	1.134911084	1.249448092
H	5.120531367	2.004170146	1.563281115
H	5.127314367	0.520483036	1.948387138
O	-1.798910128	-3.467212252	0.884225062
H	-2.420342175	-4.173117303	1.001618071
H	-1.166579083	-3.529341254	1.596155114
O	4.881255349	-0.954130070	3.190952231
H	3.984267288	-1.150213080	2.932180212
H	5.365362387	-1.768672125	3.152018227
O	0.255287017	-3.371531242	3.021043217
H	0.900819066	-2.697098193	2.828276201
H	0.722873051	-4.081597293	3.439601249

LIIC path connecting T2-MIN and T₂/T₁

Coord_1

C	-0.523438036	-0.197572014	0.062985005
N	0.271008021	-0.896583066	0.906102065
C	1.572471114	-0.637488047	1.239901088
C	1.455305106	0.887513063	-0.590476041
N	0.075146006	0.738650052	-0.601153044
N	2.128303153	0.368422027	0.527469038
H	3.093328221	0.593078042	0.693032052
N	-1.848773135	-0.461649036	0.022822002
H	-2.079924150	-1.386961102	0.338974023
H	-2.286014166	-0.202093014	-0.843988059
H	1.830797132	1.825770133	-0.963882071
O	2.142177154	-1.268604091	2.107309152
O	-2.780555198	0.430916030	-2.795451199

H	-2.482203181	-0.043150002	-3.559686256
H	-2.438437174	1.317243095	-2.865619208
O	-1.346122097	2.912755211	-2.305690167
H	-1.696506123	3.669207262	-1.853003134
H	-0.897228064	2.382873172	-1.657166118
O	4.911818351	1.134911084	1.249448092
H	5.120531367	2.004170146	1.563281115
H	5.127314367	0.520483036	1.948387138
O	-1.798910128	-3.467212252	0.884225062
H	-2.420342175	-4.173117303	1.001618071
H	-1.166579083	-3.529341254	1.596155114
O	4.881255349	-0.954130070	3.190952231
H	3.984267288	-1.150213080	2.932180212
H	5.365362387	-1.768672125	3.152018227
O	0.255287017	-3.371531242	3.021043217
H	0.900819066	-2.697098193	2.828276201
H	0.722873051	-4.081597293	3.439601249

Coord_2

C	-0.519397037	-0.193336014	0.063167004
N	0.273756017	-0.898478065	0.906533064
C	1.576031111	-0.632209044	1.236917090
C	1.457609107	0.891582065	-0.592523041
N	0.076008004	0.745497055	-0.601279041
N	2.129803154	0.377546027	0.527399039
H	3.095267221	0.601468042	0.691392047
N	-1.846094133	-0.456909031	0.025160002
H	-2.079257148	-1.383086101	0.338754022
H	-2.286232166	-0.194846016	-0.839441062
H	1.835281131	1.825859130	-0.973400070
O	2.147362154	-1.263591089	2.104115149
O	-2.782710198	0.437616033	-2.794138199
H	-2.485993180	-0.037147005	-3.558571259
H	-2.437942177	1.322762096	-2.864026204
O	-1.343110099	2.915438208	-2.305135166
H	-1.693410124	3.671470262	-1.851782132
H	-0.893833064	2.384769171	-1.657202118
O	4.915454355	1.137346082	1.247461089
H	5.126540371	2.006294147	1.560595112
H	5.132217368	0.522507039	1.945605142
O	-1.815219133	-3.499016254	0.887184063
H	-2.416936174	-4.223410303	0.994469072
H	-1.177855082	-3.555178254	1.594071113
O	4.888109353	-0.952067067	3.189405229
H	3.991156287	-1.149596081	2.932064211
H	5.372602389	-1.766557125	3.153780228
O	0.250720016	-3.376672242	3.010048216

H	0.884640064	-2.693412193	2.816321203
H	0.698469052	-4.065668291	3.482727252

Coord_3

C	-0.514026037	-0.197913016	0.068697007
N	0.279811022	-0.910386067	0.909163064
C	1.582200112	-0.635471046	1.236178088
C	1.458522107	0.892057066	-0.587515040
N	0.075803006	0.746533052	-0.593512042
N	2.131442153	0.380916029	0.532286038
H	3.097095222	0.605427044	0.694218050
N	-1.841597132	-0.463286035	0.033278005
H	-2.074935151	-1.391475101	0.341768026
H	-2.285780164	-0.196977013	-0.827727062
H	1.836443130	1.823738130	-0.973314068
O	2.156819155	-1.268671090	2.100857153
O	-2.784867199	0.442846034	-2.792466200
H	-2.489611181	-0.032326004	-3.557203256
H	-2.437793176	1.326952095	-2.861880205
O	-1.341047096	2.917078208	-2.303683167
H	-1.691543123	3.672454267	-1.849492133
H	-0.891181065	2.385645171	-1.656466117
O	4.918812355	1.140074081	1.245877087
H	5.131984372	2.008690145	1.558544111
H	5.137104368	0.524697039	1.943027138
O	-1.829448132	-3.525354253	0.888233061
H	-2.413826172	-4.265283305	0.985102068
H	-1.188140087	-3.577037259	1.590843116
O	4.895561354	-0.950291069	3.187640227
H	3.998699285	-1.149503083	2.931736211
H	5.380724386	-1.764534128	3.155048227
O	0.245737018	-3.381319243	2.999433216
H	0.869495064	-2.691134191	2.803576202
H	0.670448048	-4.046908291	3.524575256

Coord_4

C	-0.510590036	-0.188844013	0.064215003
N	0.280756021	-0.906135064	0.907365068
C	1.584212112	-0.624342046	1.231192090
C	1.461656106	0.898364065	-0.595030045
N	0.077359004	0.756428053	-0.600011042
N	2.132718153	0.394229028	0.528364036
H	3.098827224	0.617621045	0.689256050
N	-1.839710133	-0.452831032	0.030365000
H	-2.075900148	-1.381204098	0.338074024
H	-2.285931165	-0.185495015	-0.829528058
H	1.842683130	1.825207131	-0.990009071

O	2.159431158	-1.256370090	2.097453151
O	-2.787110201	0.446479032	-2.790278200
H	-2.493176179	-0.028883002	-3.555400254
H	-2.438043175	1.329671098	-2.859103205
O	-1.339917097	2.917541211	-2.301405165
H	-1.690852123	3.672072264	-1.846251134
H	-0.889257062	2.385404174	-1.655001121
O	4.921940353	1.143017085	1.244606088
H	5.136947372	2.011299142	1.556969110
H	5.142022372	0.527018036	1.940603141
O	-1.841489132	-3.545826258	0.886938064
H	-2.410957174	-4.298656307	0.972870067
H	-1.197385088	-3.594677261	1.586144112
O	4.903639351	-0.948736066	3.185719229
H	4.006912291	-1.149856081	2.931293210
H	5.389728390	-1.762559128	3.155931228
O	0.240295018	-3.385503242	2.989173216
H	0.855344060	-2.690100195	2.790335203
H	0.638886043	-4.025356288	3.564821255

Coord_5

C	-0.505884036	-0.188537011	0.065342002
N	0.284950021	-0.911786063	0.908082066
C	1.588793115	-0.621681046	1.228679091
C	1.463383108	0.900899067	-0.595465045
N	0.077816007	0.760423055	-0.598507041
N	2.134122155	0.401716029	0.529470037
H	3.100460223	0.625273043	0.688756051
N	-1.836084131	-0.453362035	0.033590002
H	-2.073336147	-1.383006100	0.338111024
H	-2.285516163	-0.183359012	-0.823816061
H	1.845636135	1.824221131	-0.997227070
O	2.166273155	-1.254004091	2.094275151
O	-2.789510200	0.448427034	-2.787453203
H	-2.496791180	-0.026970000	-3.553011257
H	-2.438733175	1.330816095	-2.855638205
O	-1.339694096	2.916728210	-2.298376165
H	-1.691276121	3.670265262	-1.842178131
H	-0.888039065	2.383974173	-1.652855117
O	4.924874355	1.146097081	1.243570091
H	5.141503371	2.014059146	1.555728110
H	5.147000369	0.529434038	1.938286139
O	-1.851265131	-3.560165257	0.882986063
H	-2.408242172	-4.323541312	0.957279066
H	-1.205555088	-3.607946258	1.579733114
O	4.912350355	-0.947347066	3.183697227
H	4.015792287	-1.150586081	2.930820211

H	5.399594387	-1.760595129	3.156525230
O	0.234375017	-3.389258246	2.979258212
H	0.842129060	-2.690157192	2.776849200
H	0.603913042	-4.001055288	3.603159258

Coord_6

C	-0.501019034	-0.189473015	0.067002005
N	0.289558022	-0.918569068	0.909165064
C	1.593664112	-0.619817046	1.226519090
C	1.464900105	0.902774064	-0.595351044
N	0.078109007	0.763406054	-0.596376044
N	2.135477156	0.408599027	0.531022040
H	3.101994223	0.632578044	0.688627049
N	-1.832224132	-0.455502033	0.037410000
H	-2.070269147	-1.386497098	0.338656024
H	-2.284988166	-0.182863014	-0.817429061
H	1.848114135	1.822664133	-1.003796070
O	2.173607155	-1.252375093	2.091352150
O	-2.792124203	0.448634032	-2.783898201
H	-2.500541178	-0.026695003	-3.549923254
H	-2.439894174	1.330319097	-2.851449206
O	-1.340345095	2.914566209	-2.294669167
H	-1.692750123	3.666998264	-1.837383134
H	-0.887502067	2.381307172	-1.650078117
O	4.927642355	1.149243082	1.242702087
H	5.145712372	2.016909146	1.554704109
H	5.152057372	0.531907036	1.936041141
O	-1.858721133	-3.568201258	0.876168064
H	-2.405567171	-4.340001312	0.937970066
H	-1.212614085	-3.616751260	1.571446113
O	4.921686354	-0.946083067	3.181620228
H	4.025323288	-1.151641081	2.930389212
H	5.410288392	-1.758620128	3.156914228
O	0.227975015	-3.392621242	2.969686216
H	0.829781058	-2.691164196	2.763331198
H	0.565708043	-3.974058284	3.639299264

Coord_7

C	-0.496028036	-0.191606012	0.069263005
N	0.294538019	-0.926426064	0.910705065
C	1.598787114	-0.618717045	1.224776086
C	1.466198103	0.903939063	-0.594689043
N	0.078224008	0.765369053	-0.593599044
N	2.136767153	0.414859030	0.533036036
H	3.103421224	0.639497047	0.688864051
N	-1.828167132	-0.459169030	0.041920003
H	-2.066763146	-1.391573099	0.339851023

H	-2.284390163	-0.183955014	-0.810278056
H	1.850131131	1.820459130	-1.009769073
O	2.181387156	-1.251422092	2.088773152
O	-2.794999202	0.447072033	-2.779549200
H	-2.504494180	-0.028135000	-3.546050253
H	-2.441546175	1.328137098	-2.846520206
O	-1.341837095	2.911010212	-2.290356166
H	-1.695210120	3.662257265	-1.831972133
H	-0.887618062	2.377375174	-1.646723117
O	4.930261353	1.152386083	1.241949089
H	5.149620373	2.019790146	1.553801111
H	5.157200371	0.534396037	1.933840140
O	-1.863800134	-3.569827256	0.866374062
H	-2.402788175	-4.348120315	0.914702068
H	-1.218526090	-3.621044263	1.561186113
O	4.931623355	-0.944918068	3.179527231
H	4.035476289	-1.152977084	2.930058211
H	5.421761389	-1.756623124	3.157168228
O	0.221103018	-3.395635245	2.960458211
H	0.818221059	-2.693001192	2.749951200
H	0.524488040	-3.944425284	3.672971262

Coord_8

C	-0.490944034	-0.194893012	0.072172003
N	0.299846022	-0.935305066	0.912771063
C	1.604122115	-0.618353045	1.223502087
C	1.467265104	0.904356066	-0.593485043
N	0.078144007	0.766311057	-0.590163043
N	2.137972153	0.420483030	0.535520036
H	3.104727223	0.645995048	0.689460048
N	-1.823956130	-0.464283031	0.047188005
H	-2.062883150	-1.398139098	0.341799025
H	-2.283761162	-0.186577013	-0.802302058
H	1.851701131	1.817543131	-1.015185075
O	2.189560156	-1.251101088	2.086607150
O	-2.798174202	0.443730030	-2.774363200
H	-2.508709183	-0.031339004	-3.541335257
H	-2.443702176	1.324248095	-2.840847203
O	-1.344135094	2.906027209	-2.285504166
H	-1.698598124	3.656038263	-1.826038130
H	-0.888364064	2.372162169	-1.642840120
O	4.932736358	1.155462085	1.241271091
H	5.153260372	2.022644147	1.552944113
H	5.162422372	0.536856040	1.931662142
O	-1.866438135	-3.564970255	0.853569062
H	-2.399737172	-4.347968314	0.887328062
H	-1.223243086	-3.620798259	1.548907110

O	4.942126354	-0.943840070	3.177455227
H	4.046207289	-1.154567082	2.929877212
H	5.433956389	-1.754605128	3.157349227
O	0.213773014	-3.398351247	2.951580210
H	0.807364057	-2.695569194	2.736846200
H	0.480502033	-3.912220282	3.703923268

Coord_9

C	-0.485805035	-0.199297016	0.075761005
N	0.305433022	-0.945162066	0.915412065
C	1.609621114	-0.618704043	1.222731086
C	1.468088107	0.903992066	-0.591745045
N	0.077854007	0.766234057	-0.586068042
N	2.139067153	0.425453031	0.538481037
H	3.105892222	0.652036045	0.690410048
N	-1.819632132	-0.470777036	0.053256001
H	-2.058691151	-1.406109101	0.344571025
H	-2.283141162	-0.190675014	-0.793463057
H	1.852830136	1.813861132	-1.020080076
O	2.198068156	-1.251378091	2.084904152
O	-2.801678202	0.438609034	-2.768319202
H	-2.513232182	-0.036338004	-3.535741256
H	-2.446374177	1.318645097	-2.834436205
O	-1.347210096	2.899604209	-2.280174166
H	-1.702864124	3.648347264	-1.819664132
H	-0.889721065	2.365662168	-1.638473117
O	4.935065357	1.158409083	1.240641090
H	5.156650371	2.025414146	1.552080110
H	5.167707371	0.539242036	1.929495140
O	-1.866551136	-3.553567258	0.837787060
H	-2.396216175	-4.339575314	0.855780060
H	-1.226703090	-3.615991261	1.534609111
O	4.953149354	-0.942851070	3.175431230
H	4.057469293	-1.156399083	2.929883212
H	5.446808390	-1.752580125	3.157506229
O	0.206004015	-3.400830247	2.943054212
H	0.797121058	-2.698793196	2.724117195
H	0.434029031	-3.877506281	3.731924270

Coord_10

C	-0.481122033	-0.200337013	0.087795009
N	0.310631025	-0.959914067	0.918946064
C	1.616299119	-0.629660044	1.222086088
C	1.469722106	0.906628067	-0.578271044
N	0.078042008	0.772841057	-0.567760038
N	2.142450157	0.423339032	0.547989040
H	3.110320224	0.647317049	0.697115052

N	-1.816529132	-0.470197031	0.069111004
H	-2.057527146	-1.408435099	0.350851025
H	-2.285070167	-0.180279015	-0.771549055
H	1.856139134	1.815258133	-1.007523070
O	2.208162160	-1.270138091	2.077192150
O	-2.810984202	0.463666032	-2.743277195
H	-2.526741183	-0.006348000	-3.515281252
H	-2.452660178	1.342722096	-2.803558199
O	-1.348297095	2.915883209	-2.241722163
H	-1.701981123	3.660939264	-1.773874128
H	-0.888927061	2.376021173	-1.606024116
O	4.943400354	1.141648082	1.244711087
H	5.169183373	2.005572143	1.561671114
H	5.179072373	0.516277035	1.926856138
O	-1.872232134	-3.532496256	0.805691057
H	-2.402457175	-4.318351311	0.802108056
H	-1.235569090	-3.610496258	1.502823106
O	4.969427360	-0.975730069	3.162556226
H	4.072799293	-1.187898083	2.919762211
H	5.462683396	-1.785603130	3.139610227
O	0.195038012	-3.421536249	2.917383210
H	0.786087057	-2.721068198	2.698070197
H	0.383311027	-3.865308280	3.735569269

LIIC path connecting T₂/T₁ and T1-MIN
Coord_1

C	-0.481122033	-0.200337013	0.087795009
N	0.310631025	-0.959914067	0.918946064
C	1.616299119	-0.629660044	1.222086088
C	1.469722106	0.906628067	-0.578271044
N	0.078042008	0.772841057	-0.567760038
N	2.142450157	0.423339032	0.547989040
H	3.110320224	0.647317049	0.697115052
N	-1.816529132	-0.470197031	0.069111004
H	-2.057527146	-1.408435099	0.350851025
H	-2.285070167	-0.180279015	-0.771549055
H	1.856139134	1.815258133	-1.007523070
O	2.208162160	-1.270138091	2.077192150
O	-2.810984202	0.463666032	-2.743277195
H	-2.526741183	-0.006348000	-3.515281252
H	-2.452660178	1.342722096	-2.803558199
O	-1.348297095	2.915883209	-2.241722163
H	-1.701981123	3.660939264	-1.773874128
H	-0.888927061	2.376021173	-1.606024116
O	4.943400354	1.141648082	1.244711087
H	5.169183373	2.005572143	1.561671114
H	5.179072373	0.516277035	1.926856138

O	-1.872232134	-3.532496256	0.805691057
H	-2.402457175	-4.318351311	0.802108056
H	-1.235569090	-3.610496258	1.502823106
O	4.969427360	-0.975730069	3.162556226
H	4.072799293	-1.187898083	2.919762211
H	5.462683396	-1.785603130	3.139610227
O	0.195038012	-3.421536249	2.917383210
H	0.786087057	-2.721068198	2.698070197
H	0.383311027	-3.865308280	3.735569269

Coord_2

C	-0.475291034	-0.197114017	0.084677007
N	0.313662025	-0.969085069	0.913469064
C	1.618891119	-0.631777045	1.213929085
C	1.469805108	0.914165064	-0.579592040
N	0.079036004	0.773652058	-0.576467042
N	2.145392154	0.418706032	0.538964038
H	3.110587226	0.649709046	0.694440050
N	-1.810507132	-0.467624034	0.072133003
H	-2.048516146	-1.407762102	0.348816026
H	-2.284848166	-0.171772015	-0.763080054
H	1.854057134	1.828596130	-0.998178070
O	2.210225157	-1.270892089	2.071149147
O	-2.822596203	0.466892034	-2.738510197
H	-2.537748181	-0.005480001	-3.508844250
H	-2.461264177	1.344717099	-2.799800200
O	-1.347692097	2.910387211	-2.241486160
H	-1.696023122	3.651109262	-1.762982126
H	-0.885298064	2.361968173	-1.614981118
O	4.939923357	1.143572080	1.248276091
H	5.169496371	2.007102142	1.563586111
H	5.178783373	0.517678037	1.928797139
O	-1.871911135	-3.533481256	0.799198058
H	-2.392378174	-4.325611311	0.781949054
H	-1.235197089	-3.615377262	1.496578106
O	4.974533359	-0.976978070	3.162983229
H	4.078576294	-1.192688085	2.921413212
H	5.470159395	-1.785524129	3.143268228
O	0.193829017	-3.439824249	2.917251212
H	0.779796055	-2.737430200	2.687927192
H	0.355196025	-3.815522273	3.774179274

Coord_3

C	-0.469467031	-0.194020013	0.081649007
N	0.316492022	-0.978428069	0.907990063
C	1.621167116	-0.634139043	1.205769087
C	1.469741104	0.921377068	-0.580710043

N	0.079968006	0.774278053	-0.585033040
N	2.148103156	0.413861028	0.530031039
H	3.110526222	0.651779045	0.691991049
N	-1.804361130	-0.465125032	0.075202003
H	-2.039254148	-1.407098101	0.346941024
H	-2.284296166	-0.163242011	-0.754508055
H	1.851854132	1.841478130	-0.988531073
O	2.212301162	-1.271834094	2.064850149
O	-2.833830202	0.469924034	-2.733637195
H	-2.548268182	-0.004837998	-3.502229254
H	-2.469492179	1.346543100	-2.795913202
O	-1.346850096	2.904698207	-2.240919163
H	-1.689685123	3.641042263	-1.751912124
H	-0.881867064	2.347690171	-1.623606115
O	4.936092358	1.145697082	1.251603092
H	5.169292373	2.008904144	1.565126112
H	5.178428375	0.519416035	1.930505138
O	-1.871131133	-3.534370253	0.793103058
H	-2.381825173	-4.332394310	0.762641054
H	-1.234656090	-3.619826261	1.491111107
O	4.980164361	-0.977807069	3.163339228
H	4.084901296	-1.197280084	2.923173208
H	5.478331394	-1.784897128	3.146830226
O	0.192274013	-3.457496251	2.918341211
H	0.774812057	-2.754729200	2.678891194
H	0.323213023	-3.764850271	3.806972272

Coord_4

C	-0.463666032	-0.191007015	0.078746004
N	0.319074021	-0.987899072	0.902580067
C	1.623103116	-0.636728048	1.197665087
C	1.469548107	0.928202068	-0.581662043
N	0.080844006	0.774717054	-0.593475042
N	2.150588156	0.408768030	0.521186038
H	3.110152226	0.653467046	0.689747052
N	-1.798134132	-0.462577032	0.078365007
H	-2.029806148	-1.406299102	0.345252023
H	-2.283483164	-0.154568012	-0.745781054
H	1.849583131	1.853807135	-0.978658071
O	2.214316158	-1.272878092	2.058458149
O	-2.844822203	0.472797033	-2.728610196
H	-2.558487182	-0.004432002	-3.495380251
H	-2.477434177	1.348211098	-2.791896202
O	-1.345754096	2.898786207	-2.240109162
H	-1.682922122	3.630739261	-1.740771128
H	-0.878612063	2.333170167	-1.631965115
O	4.931934353	1.147954081	1.254647089

H	5.168614370	2.010928147	1.566193114
H	5.178020374	0.521463035	1.931974139
O	-1.869877136	-3.535009256	0.787345059
H	-2.370663169	-4.338653312	0.744059053
H	-1.233819090	-3.623774262	1.486240109
O	4.986299361	-0.978164068	3.163707229
H	4.091751294	-1.201614088	2.925139212
H	5.487163394	-1.783678126	3.150429229
O	0.190618011	-3.474939250	2.920392212
H	0.771096058	-2.772882202	2.671210192
H	0.287453019	-3.713597269	3.834035275

Coord_5

C	-0.457879034	-0.188057016	0.076030007
N	0.321409021	-0.997470073	0.897335064
C	1.624727118	-0.639528047	1.189693084
C	1.469266104	0.934568065	-0.582466044
N	0.081692008	0.774941054	-0.601779045
N	2.152888157	0.403394029	0.512436039
H	3.109509223	0.654728049	0.687697051
N	-1.791852131	-0.459888034	0.081711005
H	-2.020247143	-1.405246102	0.343824027
H	-2.282459164	-0.145662012	-0.736802054
H	1.847304134	1.865488135	-0.968629072
O	2.216218158	-1.273955094	2.052164146
O	-2.855681206	0.475507034	-2.723335198
H	-2.568566183	-0.004314001	-3.488189251
H	-2.485158181	1.349694096	-2.787707203
O	-1.344374097	2.892587207	-2.239117161
H	-1.675672118	3.620168263	-1.729648123
H	-0.875495061	2.318358168	-1.640096119
O	4.927503356	1.150333082	1.257357090
H	5.167520370	2.013181145	1.566677115
H	5.177611373	0.523851038	1.933189141
O	-1.868234136	-3.535282253	0.781909054
H	-2.358875169	-4.344349313	0.726138053
H	-1.232626087	-3.627201262	1.481793105
O	4.992996359	-0.977931071	3.164169227
H	4.099184293	-1.205586087	2.927412209
H	5.496711398	-1.781749127	3.154193225
O	0.189122011	-3.492568251	2.923043210
H	0.768506058	-2.791771200	2.664928191
H	0.247627017	-3.661929265	3.855131275

Coord_6

C	-0.452060032	-0.185184012	0.073601004
N	0.323562021	-1.007139073	0.892379065

C	1.626138117	-0.642530048	1.181956084
C	1.468958107	0.940398069	-0.583125044
N	0.082562007	0.774890058	-0.609903043
N	2.155086158	0.397710030	0.503811037
H	3.108683225	0.655542046	0.685840052
N	-1.785517128	-0.457003034	0.085386004
H	-2.010670146	-1.403857102	0.342794026
H	-2.281248163	-0.136468007	-0.727417053
H	1.845081134	1.876422133	-0.958499069
O	2.217986161	-1.275023090	2.046199149
O	-2.866483206	0.478005036	-2.717671197
H	-2.578632188	-0.004593999	-3.480493251
H	-2.492700179	1.350919099	-2.783264199
O	-1.342650096	2.885995209	-2.237976159
H	-1.667850122	3.609261259	-1.718606126
H	-0.872457065	2.303168166	-1.648003117
O	4.922884353	1.152887082	1.259677093
H	5.166082373	2.015746147	1.566457115
H	5.177309371	0.526687036	1.934130140
O	-1.866426133	-3.535120256	0.776853056
H	-2.346625170	-4.349462313	0.708911053
H	-1.231127086	-3.630148260	1.477628104
O	5.000406359	-0.976917072	3.164805229
H	4.107358298	-1.209034089	2.930105213
H	5.507141397	-1.778905127	3.158248225
O	0.188050015	-3.510815251	2.925827212
H	0.766770055	-2.811247203	2.659832193
H	0.203064017	-3.609869262	3.869579280

Coord_7

C	-0.446120033	-0.182452013	0.071606006
N	0.325681021	-1.016940076	0.887870062
C	1.627521116	-0.645727046	1.174583084
C	1.468714108	0.945604067	-0.583610040
N	0.083536005	0.774460053	-0.617759044
N	2.157315153	0.391699026	0.495371036
H	3.107807225	0.655928049	0.684194051
N	-1.779103129	-0.453917031	0.089605007
H	-2.001188142	-1.402100101	0.342380024
H	-2.279839165	-0.126975007	-0.717406052
H	1.842978131	1.886514136	-0.948302066
O	2.219643157	-1.276075089	2.040829148
O	-2.877250206	0.480183035	-2.711413195
H	-2.588763186	-0.005454002	-3.472062251
H	-2.500045180	1.351750098	-2.778435203
O	-1.340490095	2.878855206	-2.236688163

H	-1.659339121	3.597909258	-1.707687125
H	-0.869405062	2.287468165	-1.655653121
O	4.918199356	1.155763081	1.261550089
H	5.164386371	2.018801145	1.565411111
H	5.177279372	0.530179040	1.934777138
O	-1.864880137	-3.534510252	0.772337058
H	-2.334351169	-4.353982313	0.692552051
H	-1.229531088	-3.632735260	1.473656105
O	5.008796358	-0.974832071	3.165701227
H	4.116549297	-1.211727088	2.933340211
H	5.518760399	-1.774829129	3.162720228
O	0.187639013	-3.530092252	2.928168212
H	0.765464056	-2.831147205	2.655352189
H	0.152714013	-3.557306255	3.876075280

Coord_8

C	-0.439915033	-0.179982014	0.070243004
N	0.328017021	-1.026952072	0.883998061
C	1.629169117	-0.649120046	1.167734086
C	1.468656105	0.950094067	-0.583858044
N	0.084730004	0.773501057	-0.625207044
N	2.159774155	0.385363029	0.487209037
H	3.107067223	0.655956047	0.682802051
N	-1.772546126	-0.450693034	0.094668005
H	-1.991945146	-1.400007099	0.342910027
H	-2.278174162	-0.117232007	-0.706469053
H	1.841055132	1.895678136	-0.938042066
O	2.221267160	-1.277155093	2.036349144
O	-2.887923208	0.481852033	-2.704294194
H	-2.598949186	-0.007170002	-3.462584247
H	-2.507105183	1.351978099	-2.773029202
O	-1.337746094	2.870954209	-2.235211161
H	-1.649973117	3.585952260	-1.696903122
H	-0.866200063	2.271077165	-1.662958121
O	4.913610352	1.159226085	1.262935089
H	5.162523371	2.022653148	1.563430115
H	5.177754372	0.534662039	1.935117140
O	-1.864310133	-3.533517256	0.768675056
H	-2.322909166	-4.357912316	0.677454048
H	-1.228290088	-3.635181260	1.469887104
O	5.018567362	-0.971267068	3.166943227
H	4.127178298	-1.213342090	2.937251212
H	5.532038398	-1.769058128	3.167729230
O	0.188062011	-3.550733255	2.929383209
H	0.763980053	-2.851310207	2.650425189
H	0.095214005	-3.504003252	3.872474276

Coord_9

C	-0.433239033	-0.177968013	0.069762003
N	0.330954024	-1.037317072	0.880974062
C	1.631499116	-0.652723050	1.161596085
C	1.468940104	0.953780067	-0.583758040
N	0.086302004	0.771801054	-0.632047047
N	2.162730155	0.378729030	0.479466037
H	3.106711225	0.655768047	0.681748051
N	-1.765727127	-0.447488030	0.100965008
H	-1.983116141	-1.397698098	0.344851023
H	-2.276117165	-0.107366010	-0.694215049
H	1.839353134	1.903856137	-0.927672065
O	2.223014159	-1.278386091	2.033066145
O	-2.898315207	0.482729033	-2.695978195
H	-2.609047190	-0.010132003	-3.451665246
H	-2.513676183	1.351299096	-2.766800198
O	-1.334202093	2.862016204	-2.233453160
H	-1.639535117	3.573173259	-1.686231120
H	-0.862642060	2.253761162	-1.669768119
O	4.909310353	1.163697083	1.263831092
H	5.160576374	2.027771144	1.560455112
H	5.179035373	0.540634037	1.935166142
O	-1.865822136	-3.532303255	0.766406055
H	-2.313765168	-4.361258315	0.664338046
H	-1.228211087	-3.637833263	1.466494104
O	5.030269360	-0.965667071	3.168627228
H	4.139829297	-1.213458085	2.941981210
H	5.547635400	-1.760960129	3.173388230
O	0.189360014	-3.572873258	2.928699210
H	0.761517055	-2.871645208	2.643305188
H	0.029059001	-3.449626247	3.855532275

Coord_10

C	-0.423898028	-0.152036010	0.053306003
N	0.319811022	-0.996880072	0.905004064
C	1.620508115	-0.606153044	1.180635083
C	1.489371108	0.936257066	-0.624707046
N	0.107005006	0.759349053	-0.687253050
N	2.169131157	0.388648029	0.461328031
H	3.110036225	0.672011047	0.668896050
N	-1.759399125	-0.405889031	0.087894007
H	-1.987531141	-1.344138095	0.363768025
H	-2.262516162	-0.086644006	-0.720380054
H	1.870221133	1.872892134	-0.993036070
O	2.195130159	-1.198825086	2.086624153
O	-2.870002208	0.416966028	-2.755116198
H	-2.577399183	-0.113193009	-3.483789253

H	-2.472259178	1.276549089	-2.859336207
O	-1.273743090	2.788246202	-2.379464170
H	-1.571062111	3.520601251	-1.856362135
H	-0.814580060	2.190624157	-1.794270127
O	4.907009353	1.193007083	1.250597089
H	5.165241373	2.066870151	1.510222110
H	5.169779370	0.597335041	1.948988140
O	-1.908706136	-3.461944250	0.868896062
H	-2.353677172	-4.294625310	0.785986058
H	-1.276836094	-3.549353256	1.577374116
O	5.005178363	-0.855862061	3.243423235
H	4.115876295	-1.110795080	3.020890216
H	5.519218396	-1.651977117	3.290351235
O	0.129721008	-3.457999249	3.051432221
H	0.705336053	-2.771724198	2.735364196
H	-0.116294008	-3.217004231	3.935135281