

Quantum mechanics/molecular mechanics studies on mechanistic photophysics of cytosine aza-analogues: 2,4-diamino-1,3,5-triazine and 2-amino-1,3,5-triazine in aqueous solution

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1. Active Orbitals

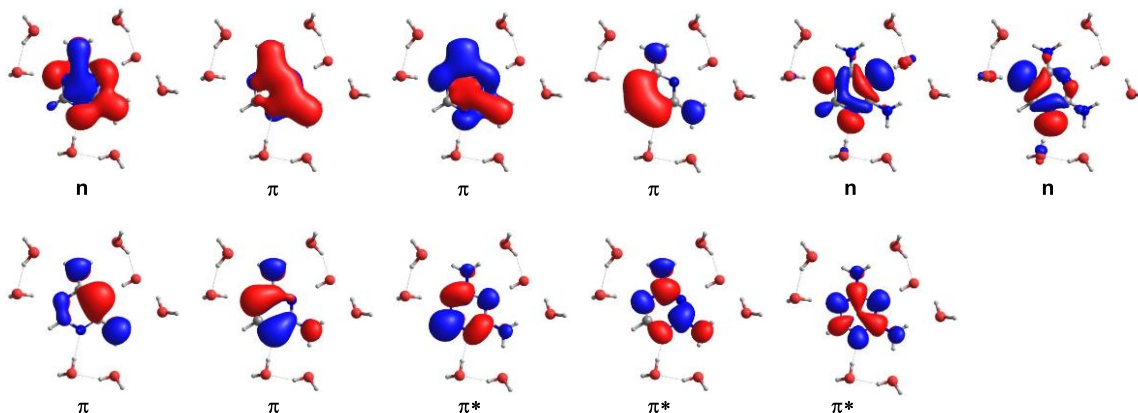


Figure S1. Molecular orbitals included in the active space for 2,4-DT used for QM/MM calculations.

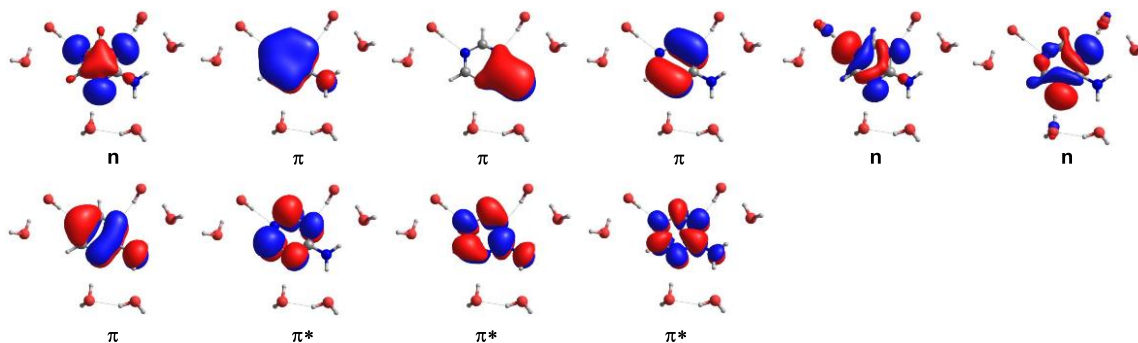


Figure S2. Molecular orbitals included in the active space for 2-AT used for QM/MM calculations.

2. The Effective Spin–Orbit Couplings Expression

Spin-orbit couplings are obtained at the QM(MS-CASPT2)/MM level within the atomic mean-field (AMFI) approximation. The effective spin–orbit couplings are expressed as follows:

$$\langle \psi_I | H_{eff}^{so} | \psi_J \rangle = \sqrt{\frac{|\langle \psi_I | H_x^{so} | \psi_J \rangle|^2 + |\langle \psi_I | H_y^{so} | \psi_J \rangle|^2 + |\langle \psi_I | H_z^{so} | \psi_J \rangle|^2}{3}}$$

in which ψ_I and ψ_J are the perturbatively modified electronic wave functions of the corresponding singlet and triplet states; H_x^{so} , H_y^{so} , H_z^{so} are the x, y, and z components of the spin–orbit operator.

3. Bond-Length Difference and Dihedral Angles of Minima and Surface Crossings

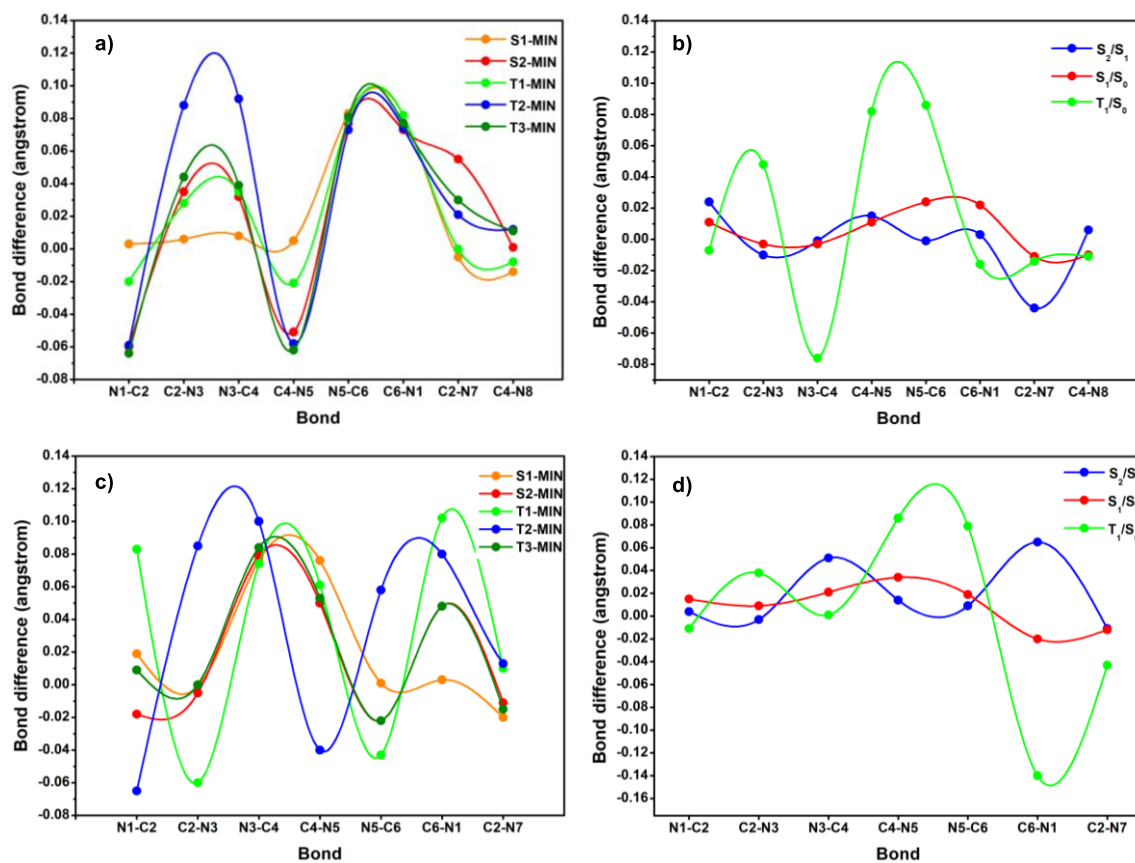


Figure S3. QM(CASSCF)/MM computed bond-length difference (in Å) of excited-state minima compared with the counterparts of the S_0 minimum S_0 -MIN (a) for 2,4-DT and (c) for 2-AT. The positive and negative values mean they are longer and shorter than those of S_0 -MIN, respectively. Bond-length difference (in Å) of surface crossings compared with the counterparts of the corresponding excited-state minimum (b) for 2,4-DT and (d) for 2-AT, respectively.

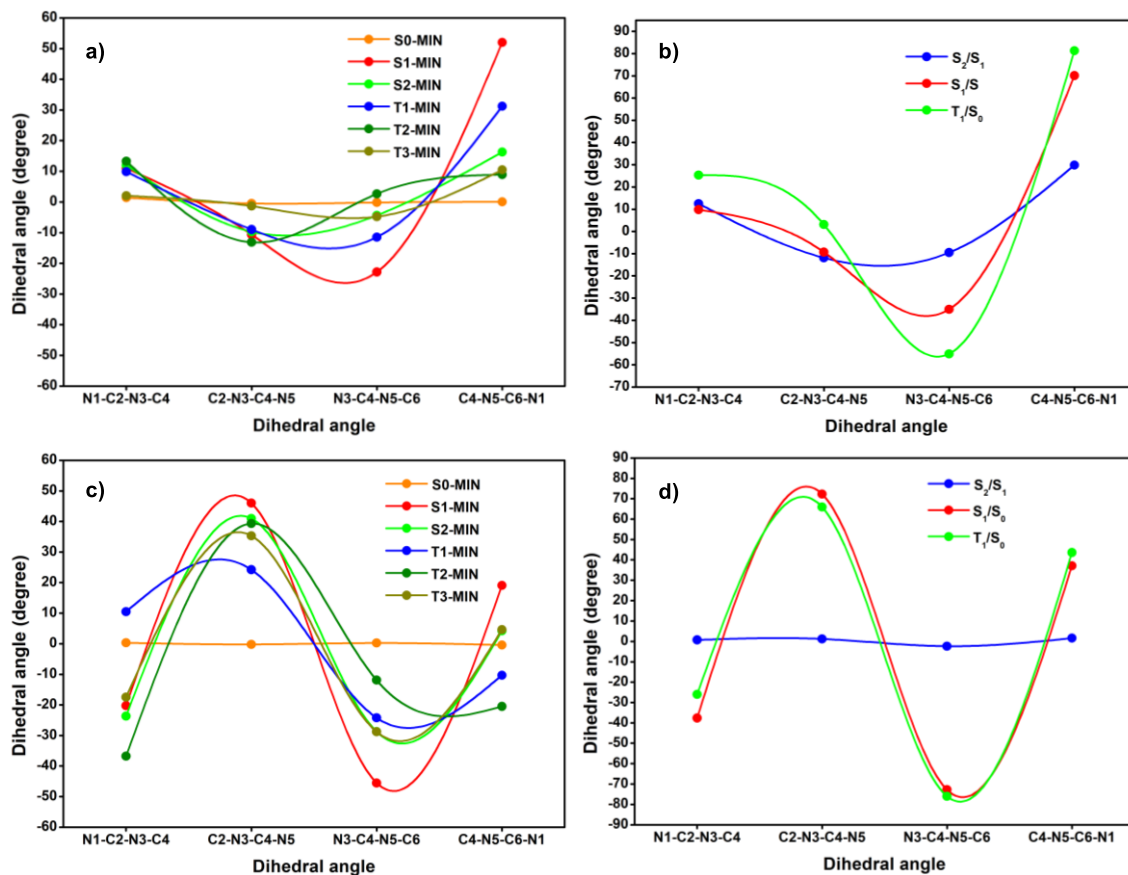


Figure S4. QM(CASSCF)/MM computed dihedal angles (in °) of minima and conical intersections and crossing points (a and b) for 2,4-DT and (c and d) for 2-AT.

4. QM(CASSCF)/MM Optimized Crossing Points

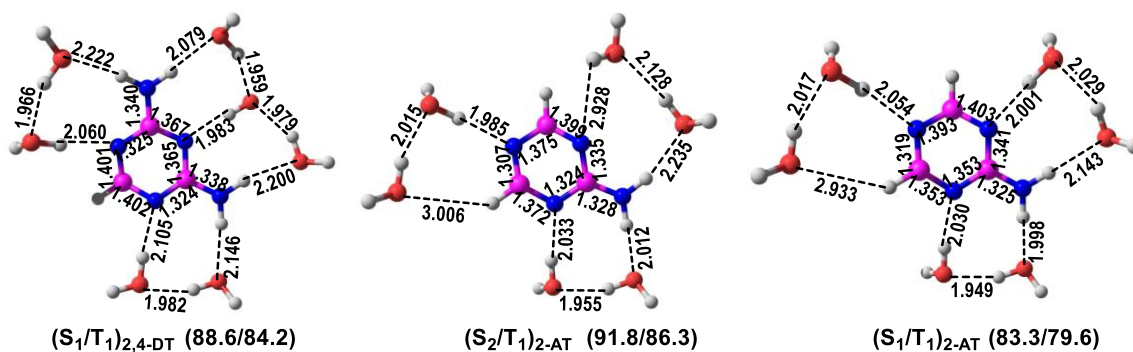


Figure S5. QM(CASSCF)/MM optimized crossing points between S₁, S₂, and T₁ states together with relative energies in kcal/mol at the QM(MS-CASPT2)/MM level.

5. The Effect of the Solvation Shell

In order to roughly estimate the effect of the explicit solvation shell, we do some computational tests in water without including explicit solvation shell of water molecules and in the gas phase. In water, we merely put the 2,4-DT and 2-AT in the QM region (referred to as QM2), respectively, and all solvent water molecules in the MM region. The computed results are given in the following tables S1 and S2. One can see that the QM2(MS-CASPT2)/MM and MS-CASPT2 computations obtain similar numbers and will give virtually the same excited-state relaxation pathways. The $S_3(\pi\pi^*)$ state is the first spectroscopic bright state at the Franck-Condon region and there are two dark states of $1n\pi^*$ character below the S_3 state. These surface crossings are all energetically accessible considering the vertical excitation energy at the Franck-Condon region. Therefore, $1n\pi^*$ state will participate in the excited-state decay processes. Differently, extending the QM region to include the explicit solvation shell of 6-7 water molecules significantly stabilizes the first bright $1\pi\pi^*$ state (S_1) and changes the order of $1n\pi^*$ state at the Franck-Condon region, due to the hydrogen-bonding interactions. In summary, the gas phase 2,4-DT and 2-AT may exhibit much more complex excited-state dynamics compared with that in water and further gas phase experiments are needed.

Table S1 QM2(MS-CASPT2)/MM and MS-CASPT2 calculated vertical excitation energies (in kcal/mol [eV]) of the low-lying excited singlet and triplet states at the S0-MIN of 2,4-DT and 2-AT in water and in the gas phase.

2,4-DT	$S_1(n\pi^*)$	$S_2(n\pi^*)$	$S_3(\pi\pi^*)$	$T_1(\pi\pi^*)$	$T_2(n\pi^*)$	$T_3(n\pi^*)$
Water	110.2 [4.78]	112.8 [4.89]	113.9 [4.94]	104.5 [4.53]	108.0 [4.69]	108.6 [4.71]
Gas	109.9 [4.77]	112.6 [4.88]	113.8 [4.93]	104.0 [4.51]	107.9 [4.68]	108.5 [4.71]
2-AT	$S_1(n\pi^*)$	$S_2(n\pi^*)$	$S_3(\pi\pi^*)$	$T_1(n\pi^*)$	$T_2(n\pi^*)$	$T_3(\pi\pi^*)$
Water	102.3 [4.44]	102.7 [4.45]	113.5 [4.92]	94.4 [4.09]	99.7 [4.32]	107.4 [4.66]
Gas	102.2 [4.43]	102.4 [4.44]	113.5 [4.92]	94.4 [4.09]	99.6 [4.32]	107.1 [4.65]

Table S2 QM2(MS-CASPT2)/MM and MS-CASPT2 calculated adiabatic excitation energies (in kcal/mol) of the optimized minima and surface crossings of 2,4-DT and 2-AT in water and in the gas phase.

2,4-DT	S0-MIN	S1-MIN	S2-MIN	T1-MIN	T2-MIN	S_2/S_1	S_1/S_0	T_1/S_0
Water	0.0	86.7	102.5	83.4	90.2	104.9/95.9	104.5/99.5	94.3/91.7
Gas	0.0	86.6	102.8	84.2	89.4	103.9/95.2	100.7/97.2	95.6/93.0
2-AT	S0-MIN	S1-MIN	S2-MIN	T1-MIN	T2-MIN	S_2/S_1	S_1/S_0	T_1/S_0
Water	0.0	85.3	94.5	82.3	83.3	98.2/89.7	108.1/101.6	100.2/95.7
Gas	0.0	84.3	91.9	83.8	83.8	96.9/88.9	107.7/100.1	97.1/95.9

6. Cartesian Coordinates of All Computed Structures

In xyz format (unit: Ångstrom)

CASSCF/ANO-L-VDZP

For 2,4-DT

S0-MIN

C	-0.724575054	-0.309980020	-0.139502008
N	0.596051045	-0.422714031	0.010687999
C	1.291079095	0.718973051	0.047564002
C	-0.585017043	1.924243140	-0.179204013
N	-1.364910096	0.864947061	-0.241782016
N	0.723508053	1.932063141	-0.030508000
N	-1.479571105	-1.423341101	-0.151859011
H	-1.025196072	-2.298364163	-0.328535022
H	-2.398063173	-1.320673095	-0.540962037
H	-1.068956077	2.887504206	-0.270127020
N	2.619836188	0.670232048	0.167373012
H	3.142204227	1.522697109	0.228523015
H	3.112959226	-0.196570012	0.195986012
O	4.196028301	3.388554245	0.450144034
H	3.509951252	4.037529291	0.319436021
H	4.934617355	3.657894262	-0.078955008
O	-0.154320013	-4.218779304	-0.696605052
H	0.730803052	-4.073099294	-0.379006028
H	-0.091825006	-4.624088335	-1.550617109
O	-4.089339294	-0.773988054	-1.965449140
H	-4.234864308	0.167451012	-1.951386139
H	-4.873874353	-1.176264085	-2.312571165
O	1.704712122	4.665816337	-0.139021012
H	1.354118097	3.778486274	-0.097140009
H	1.048312074	5.256706380	0.199363015
O	2.076288152	-2.969283216	0.563773042
H	2.057823147	-3.110214224	1.502694109
H	1.587190115	-2.162249154	0.401539030
O	-3.845299278	2.013992146	-1.364224097
H	-4.393147319	2.444727176	-0.722446052
H	-3.116447223	1.616960114	-0.894529064
O	4.683892339	-1.866649134	0.208595015
H	5.408847389	-2.179117155	-0.315210022
H	3.988624285	-2.514204180	0.170493014

S1-MIN

C	-0.650393045	-0.411435031	-0.113881008
N	0.667911050	-0.576125040	0.077044006

C	1.328062097	0.592721044	0.059158005
C	-0.580228042	1.789910130	0.608397046
N	-1.260884088	0.788815055	-0.094298005
N	0.717123053	1.790534131	0.085353004
N	-1.417312100	-1.475636106	-0.340000023
H	-0.989652072	-2.362711169	-0.527389037
H	-2.358813170	-1.326130098	-0.649611048
H	-1.071411079	2.748052200	0.677246049
N	2.654982193	0.593229043	-0.026485004
H	3.156471227	1.454190103	0.090558007
H	3.170841226	-0.263230020	-0.032347002
O	4.079873292	3.338533241	0.435365029
H	3.393767244	3.992053285	0.334504025
H	4.841813350	3.666051265	-0.023349004
O	-0.136873008	-4.235285305	-0.766947054
H	0.728066052	-4.091696297	-0.394011028
H	-0.019987004	-4.627597336	-1.621099116
O	-4.051770292	-0.709232052	-1.926949141
H	-4.147753297	0.238829017	-1.907439138
H	-4.839022348	-1.067751077	-2.313688168
O	1.566507112	4.616540331	-0.112995006
H	1.201576088	3.744312272	-0.226090017
H	0.872186063	5.247531378	-0.237589017
O	2.080192152	-3.070618219	0.576768043
H	2.054780150	-3.232068235	1.511974110
H	1.605238113	-2.246189160	0.431254031
O	-3.668946266	2.075065149	-1.389238099
H	-4.145475300	2.530207183	-0.708835052
H	-2.879247210	1.721269126	-0.990870074
O	4.614780335	-1.885520134	0.110130009
H	5.375323386	-2.264812161	-0.308118020
H	3.940678286	-2.555113185	0.171456011

S2-MIN

C	-1.204743086	-0.249190016	-0.254896018
N	0.139771010	-0.346801025	-0.036072002
C	1.031268074	0.696066048	-0.030865004
C	-0.828919060	2.018206144	0.004340000
N	-1.679436119	0.950902068	-0.279431020
N	0.555205038	1.886513136	-0.013285000
N	-1.927218137	-1.379876101	-0.361927028
H	-1.410365104	-2.207396160	-0.593549042
H	-2.823560205	-1.274758094	-0.801840060
H	-1.207780088	2.995694214	-0.241110020
N	2.377687171	0.360387027	0.048365001
H	2.944723210	1.184303086	0.180074012
H	2.684253194	-0.116943007	-0.785702059

O	4.000766289	3.098498224	0.362273025
H	3.351454242	3.790797271	0.269778017
H	4.799267346	3.410017245	-0.042049001
O	0.232528019	-3.703614266	-0.459321031
H	1.029473073	-3.406716243	-0.031672004
H	0.476727036	-4.410813319	-1.041736073
O	-4.500601326	-0.689627051	-1.976718145
H	-4.615934333	0.255714020	-1.926180140
H	-5.273462380	-1.049606076	-2.388797173
O	1.573898114	4.619031332	-0.016113003
H	1.235707089	3.728305269	-0.045202003
H	1.113620082	5.061909366	0.682377047
O	2.518349183	-2.524522184	1.067248078
H	2.294854167	-2.735370197	1.965744141
H	2.480204177	-1.574843114	0.987861072
O	-4.197167303	2.081850149	-1.386915101
H	-4.693914337	2.525527182	-0.712764051
H	-3.406090247	1.746184124	-0.974364072
O	5.460831392	-2.260900165	0.505933038
H	5.829784422	-1.846694135	1.273356092
H	4.576827330	-2.521003182	0.734185050

T1-MIN

C	-0.731234051	-0.314892023	-0.147504009
N	0.612614044	-0.457730033	0.071083004
C	1.304521092	0.719073050	0.055041006
C	-0.640272049	1.956903140	0.246679017
N	-1.362549097	0.844774062	-0.189412011
N	0.742697052	1.915476139	0.037107004
N	-1.439955103	-1.436603104	-0.312212021
H	-0.967002069	-2.305846168	-0.468877036
H	-2.377382169	-1.345109098	-0.658476048
H	-1.102198082	2.909950211	0.040022003
N	2.637389188	0.644079045	0.049031003
H	3.175752229	1.486971110	0.132770011
H	3.115468224	-0.232716014	0.071452005
O	4.159411300	3.357752239	0.421177030
H	3.469404252	4.006867290	0.310315021
H	4.911038355	3.669411265	-0.064659004
O	-0.129604007	-4.195390304	-0.731691054
H	0.743669055	-4.097722292	-0.366190027
H	-0.047989005	-4.634456335	-1.567161111
O	-4.068419293	-0.830050060	-1.948275143
H	-4.213296302	0.112064009	-1.919583136
H	-4.860729352	-1.228902086	-2.281075164
O	1.684555120	4.668113337	-0.157044012
H	1.332056094	3.780991272	-0.148714010

H	1.021807072	5.244844380	0.193636015
O	2.080368151	-3.032182218	0.634617044
H	2.068977150	-3.183119228	1.572156116
H	1.600853117	-2.217422158	0.486030036
O	-3.835279275	1.950913139	-1.418342102
H	-4.334950310	2.437948178	-0.777909056
H	-3.056635218	1.621561114	-0.976900070
O	4.625461333	-1.854401136	0.159633011
H	5.376740385	-2.179487156	-0.317226023
H	3.971890287	-2.544037183	0.194507014

T2-MIN

C	-0.868949065	-0.261278018	-0.141704010
N	0.514247037	-0.408529027	0.174276012
C	1.265283091	0.800217057	0.099495007
C	-0.670492049	2.015187145	-0.054538002
N	-1.452087105	0.879303063	-0.227598018
N	0.717480052	1.958260141	0.021912002
N	-1.536022110	-1.440960106	-0.211059017
H	-1.000302071	-2.257212165	-0.436483032
H	-2.432726177	-1.389804102	-0.661039049
H	-1.087477080	2.939298212	-0.416218031
N	2.596837187	0.623543047	0.283345021
H	3.172867228	1.439626103	0.183465011
H	3.017307215	-0.237803016	-0.001947002
O	4.230303302	3.364632242	0.392339029
H	3.521313254	3.991483287	0.273060022
H	4.968639357	3.688911267	-0.105127008
O	-0.044006004	-4.140519296	-0.715727052
H	0.796495058	-4.096938295	-0.273480019
H	0.082355003	-4.605224330	-1.531784109
O	-4.121479298	-0.837515063	-1.991005142
H	-4.277163308	0.101922009	-1.945026143
H	-4.916545354	-1.239890087	-2.312651166
O	1.728910122	4.661428336	-0.138212011
H	1.374038096	3.776353272	-0.078655007
H	1.159146084	5.229268375	0.359270023
O	2.059009149	-3.055219220	0.928441065
H	2.017832148	-3.265798236	1.853581134
H	1.566024110	-2.248152164	0.813034059
O	-3.930782285	1.944018139	-1.400216103
H	-4.459264322	2.424842177	-0.778111054
H	-3.179164231	1.598293117	-0.924522069
O	4.474257321	-1.945389142	-0.136613012
H	5.295109381	-2.001496144	0.334273024
H	3.863627279	-2.543354184	0.279759020

T3-MIN

C	-0.953302066	-0.238963015	-0.184192011
N	0.404475027	-0.284602018	0.013516002
C	1.236324088	0.816575059	0.067104004
C	-0.678208051	2.059382150	-0.125812007
N	-1.474750105	0.924013069	-0.301661020
N	0.709961052	1.975980143	-0.037037005
N	-1.640530119	-1.407757101	-0.182961012
H	-1.119168082	-2.221520160	-0.451481032
H	-2.546453184	-1.340411094	-0.612501044
H	-1.070910075	2.975162216	-0.534582038
N	2.555289184	0.576795041	0.323160021
H	3.128087223	1.402856100	0.299416023
H	2.972010214	-0.204643013	-0.146837008
O	4.224422302	3.328565241	0.421003032
H	3.520810255	3.962499286	0.306014022
H	4.943824357	3.621054259	-0.121776010
O	0.001520998	-4.035944288	-0.672572049
H	0.856818062	-3.987667289	-0.258987019
H	0.098905006	-4.527650327	-1.477457106
O	-4.208072302	-0.818861057	-1.975136143
H	-4.359487312	0.121613007	-1.933794138
H	-4.999807362	-1.217397085	-2.309694165
O	1.746692124	4.673493339	-0.115614010
H	1.389568099	3.787703272	-0.094012005
H	1.167310083	5.220261376	0.394466031
O	2.275119163	-3.262179235	1.020082071
H	2.194939158	-3.677859262	1.870364133
H	1.988117141	-2.363441169	1.139128082
O	-4.006973289	1.967753141	-1.425212103
H	-4.496811322	2.455293179	-0.776925056
H	-3.216468232	1.652142119	-0.996120073
O	4.571109331	-1.956517142	-0.119876009
H	5.408831387	-1.895274136	0.319487023
H	4.087771294	-2.662775191	0.290675020

S₂/S₁

C	-0.789025059	-0.317905021	-0.091649007
N	0.565889042	-0.377103027	0.059545003
C	1.326984095	0.748753051	-0.026921004
C	-0.628180047	1.954016139	0.272806022
N	-1.386742102	0.843181059	-0.088530004
N	0.735123054	1.912549138	-0.009664999
N	-1.483971108	-1.473381108	-0.186063012
H	-0.987491071	-2.281777166	-0.508796035
H	-2.411234172	-1.372601100	-0.556827041
H	-1.103532080	2.909633208	0.115709008

N	2.660115192	0.639204047	-0.174864013
H	3.205586231	1.458371106	0.021879003
H	3.108771222	-0.240794016	-0.027614003
O	4.178547301	3.373412245	0.440430033
H	3.481881251	4.016615290	0.343749027
H	4.916946354	3.695589266	-0.058583007
O	-0.083121009	-4.196887304	-0.764312053
H	0.778839059	-4.210688305	-0.364352025
H	-0.029965000	-4.668492339	-1.584287113
O	-4.093464294	-0.805948058	-1.963098144
H	-4.216280301	0.138761012	-1.936255141
H	-4.890783349	-1.183985088	-2.308153164
O	1.692379122	4.695200338	-0.152873010
H	1.334596098	3.813426276	-0.203608016
H	0.996177071	5.273692382	0.123176011
O	2.162925157	-3.212838230	0.760149053
H	2.147416157	-3.390234245	1.693580122
H	1.682602123	-2.402008173	0.639251043
O	-3.826944273	1.984076143	-1.394748099
H	-4.353646312	2.441921177	-0.754117056
H	-3.069218223	1.634742115	-0.934531065
O	4.635875335	-1.878839134	0.194831014
H	5.399807391	-2.152952155	-0.294349024
H	4.045411290	-2.620206189	0.261456017

S₁/T₁

C	-0.709278053	-0.386595027	-0.108006008
N	0.631963045	-0.532978038	0.111984008
C	1.317614096	0.646670045	0.065542005
C	-0.610445042	1.827791130	0.507887035
N	-1.332162094	0.782301058	-0.082974008
N	0.731505053	1.833177133	0.103316005
N	-1.426633103	-1.497544108	-0.321838025
H	-0.960749067	-2.358216168	-0.532224040
H	-2.365179173	-1.382557099	-0.654177049
H	-1.103470081	2.785469201	0.537805040
N	2.650653190	0.587903043	-0.033996003
H	3.181993229	1.430483105	0.089626005
H	3.136389226	-0.284936019	-0.029020001
O	4.150687299	3.313381240	0.439376034
H	3.473211248	3.976927288	0.346398025
H	4.917153352	3.639178263	-0.012412001
O	-0.090384009	-4.230750304	-0.776189055
H	0.769362055	-4.090620295	-0.392184028
H	0.034221004	-4.626295332	-1.627763119
O	-4.065440295	-0.777349054	-1.950972142
H	-4.177487301	0.168721011	-1.928703141

S11

H	-4.842481347	-1.145836081	-2.348586169
O	1.654128122	4.632869333	-0.086551008
H	1.287693091	3.756496271	-0.153099011
H	0.957521070	5.258710379	-0.220539016
O	2.087775150	-3.042088221	0.607363045
H	2.071955148	-3.215032230	1.540814111
H	1.604146113	-2.222791159	0.475112035
O	-3.736803268	2.013858143	-1.411944100
H	-4.250718304	2.478941179	-0.766522056
H	-2.974694212	1.662153121	-0.960257070
O	4.632747331	-1.891164138	0.117036010
H	5.394622391	-2.271767164	-0.297527019
H	3.960383286	-2.561101186	0.184014012

S₁/S₀

C	-0.615783043	-0.442862031	-0.147472010
N	0.693131051	-0.632841045	0.062245003
C	1.331031094	0.545752038	0.067935003
C	-0.542433039	1.634818116	0.824357060
N	-1.174951085	0.794264057	-0.135785009
N	0.663439048	1.725661122	0.077424008
N	-1.405914099	-1.468414107	-0.407765028
H	-1.010745072	-2.378380171	-0.559002039
H	-2.348434168	-1.289810091	-0.700915052
H	-1.038455073	2.564064187	1.059250078
N	2.648268188	0.589514044	0.005805000
H	3.119696223	1.471618106	0.093822004
H	3.193960228	-0.248964015	-0.028405002
O	3.957864286	3.359311243	0.380991030
H	3.242652235	3.977643286	0.256165017
H	4.716882338	3.722351268	-0.055357004
O	-0.151016011	-4.234992305	-0.730240055
H	0.719874050	-4.103528293	-0.366141025
H	-0.050040006	-4.661589338	-1.569909113
O	-4.013801290	-0.612674042	-1.901106135
H	-4.052288293	0.340314026	-1.881303137
H	-4.818463346	-0.923795069	-2.293128166
O	1.399079102	4.541993327	-0.174201012
H	1.045676078	3.664118265	-0.292677019
H	0.728260054	5.165940374	-0.411824029
O	2.100053153	-3.109070223	0.581794041
H	2.071832151	-3.260906236	1.518514111
H	1.625302117	-2.285357166	0.426995033
O	-3.496148251	2.167546155	-1.425514104
H	-3.917898280	2.657195191	-0.733131051
H	-2.682875195	1.818687133	-1.068251076
O	4.594523329	-1.848372135	0.103080008

H	5.381163386	-2.212549161	-0.278971022
H	3.944761286	-2.541226183	0.173322012

T₁/S₀

C	-0.583986042	-0.586611041	-0.236456017
N	0.675116047	-0.669769050	0.043966004
C	1.257893088	0.615953047	0.105044007
C	-0.698250052	1.467863106	0.731137053
N	-1.077011076	0.704244048	-0.481340033
N	0.613009043	1.729532123	0.376378027
N	-1.441772102	-1.594841114	-0.308966021
H	-1.085941080	-2.533945180	-0.307946022
H	-2.322106166	-1.425755102	-0.761579054
H	-1.347548097	2.294313163	0.977081070
N	2.563516187	0.633873047	-0.097116006
H	3.071164219	1.493141110	0.011731002
H	3.078175220	-0.216028018	-0.208959014
O	4.007537286	3.315622237	0.340353027
H	3.255239234	3.894499279	0.236820017
H	4.738871341	3.721378270	-0.104818006
O	-0.157063009	-4.336186315	-0.717192052
H	0.730230054	-4.184146304	-0.405034029
H	-0.097712008	-4.642859337	-1.611518113
O	-3.966440286	-0.691632050	-1.862146132
H	-4.054438292	0.254635017	-1.784221131
H	-4.780329346	-1.023570074	-2.216650157
O	1.386562097	4.487513323	0.011574001
H	1.090586081	3.581021260	0.117143010
H	0.993620071	4.984803361	0.714637052
O	2.125568153	-3.178070226	0.526254037
H	2.138005152	-3.346116240	1.460483105
H	1.667466119	-2.342475167	0.407295028
O	-3.631619262	2.120906155	-1.474178107
H	-3.892265278	2.730300198	-0.797359056
H	-2.687682193	2.020712147	-1.417312100
O	4.571457329	-1.828783131	0.015413002
H	5.358238385	-2.157029154	-0.397885029
H	3.951416282	-2.546802181	0.089625004

LIIC path connecting Franck-Condon point and S1-MIN

Coord_1

C	-0.724575054	-0.309980020	-0.139502008
N	0.596051045	-0.422714031	0.010687999
C	1.291079095	0.718973051	0.047564002
C	-0.585017043	1.924243140	-0.179204013
N	-1.364910096	0.864947061	-0.241782016
N	0.723508053	1.932063141	-0.030508000

N	-1.479571105	-1.423341101	-0.151859011
H	-1.025196072	-2.298364163	-0.328535022
H	-2.398063173	-1.320673095	-0.540962037
H	-1.068956077	2.887504206	-0.270127020
N	2.619836188	0.670232048	0.167373012
H	3.142204227	1.522697109	0.228523015
H	3.112959226	-0.196570012	0.195986012
O	4.196028301	3.388554245	0.450144034
H	3.509951252	4.037529291	0.319436021
H	4.934617355	3.657894262	-0.078955008
O	-0.154320013	-4.218779304	-0.696605052
H	0.730803052	-4.073099294	-0.379006028
H	-0.091825006	-4.624088335	-1.550617109
O	-4.089339294	-0.773988054	-1.965449140
H	-4.234864308	0.167451012	-1.951386139
H	-4.873874353	-1.176264085	-2.312571165
O	1.704712122	4.665816337	-0.139021012
H	1.354118097	3.778486274	-0.097140009
H	1.048312074	5.256706380	0.199363015
O	2.076288152	-2.969283216	0.563773042
H	2.057823147	-3.110214224	1.502694109
H	1.587190115	-2.162249154	0.401539030
O	-3.845299278	2.013992146	-1.364224097
H	-4.393147319	2.444727176	-0.722446052
H	-3.116447223	1.616960114	-0.894529064
O	4.683892339	-1.866649134	0.208595015
H	5.408847389	-2.179117155	-0.315210022
H	3.988624285	-2.514204180	0.170493014

Coord_2

C	-0.716729054	-0.317866021	-0.141009010
N	0.602991046	-0.432775029	0.016802002
C	1.293320092	0.711654054	0.046532005
C	-0.598114042	1.934230138	-0.117022008
N	-1.361513101	0.855612062	-0.237257016
N	0.725582052	1.925276136	-0.027096002
N	-1.469834107	-1.430185104	-0.173259013
H	-1.014987073	-2.305926164	-0.345758027
H	-2.390896171	-1.326484096	-0.555751038
H	-1.096727077	2.890740209	-0.195039012
N	2.623209190	0.669996046	0.149212008
H	3.140785228	1.525226111	0.215448013
H	3.119575227	-0.195183012	0.179292015
O	4.204975302	3.390432242	0.455322034
H	3.518972253	4.039024290	0.322940021
H	4.950192354	3.668469266	-0.059844004
O	-0.154883010	-4.211235305	-0.702300052

H	0.727552052	-4.067048295	-0.376203029
H	-0.084862007	-4.616228333	-1.555829114
O	-4.090975293	-0.780126055	-1.956203139
H	-4.231243306	0.161633010	-1.953016142
H	-4.875239350	-1.182228087	-2.304138164
O	1.714175124	4.664486335	-0.148612011
H	1.350826096	3.782031270	-0.122234007
H	1.050836075	5.278324382	0.130349009
O	2.073281150	-2.973216214	0.571686042
H	2.052087146	-3.114283222	1.510491107
H	1.587104114	-2.163788155	0.408599027
O	-3.832845277	2.012221144	-1.395260099
H	-4.373722317	2.453342177	-0.755663053
H	-3.097651223	1.625282120	-0.928554066
O	4.675975339	-1.866453132	0.208035013
H	5.405280391	-2.190016158	-0.302760021
H	3.981891288	-2.516036181	0.180813013

Coord_3

C	-0.708667049	-0.324333022	-0.143072012
N	0.610154042	-0.442449030	0.022801004
C	1.296369095	0.704540049	0.045665001
C	-0.607969043	1.941685140	-0.051079003
N	-1.355920099	0.848827063	-0.232663017
N	0.727934054	1.918468139	-0.023074001
N	-1.460716107	-1.434645105	-0.196201017
H	-1.006204075	-2.311406165	-0.364991027
H	-2.384063170	-1.328930096	-0.572383042
H	-1.118192078	2.892700208	-0.115393010
N	2.627105189	0.669152050	0.131127011
H	3.140589226	1.526627108	0.202798015
H	3.126306224	-0.194633011	0.162315014
O	4.210081302	3.391600242	0.458736031
H	3.524386255	4.040177294	0.325250022
H	4.961227356	3.677487266	-0.043395006
O	-0.155331012	-4.203793300	-0.708230049
H	0.724265051	-4.060962291	-0.373549025
H	-0.077586005	-4.608574334	-1.561150113
O	-4.092609297	-0.786264056	-1.946957142
H	-4.227620305	0.155816013	-1.954645140
H	-4.876603352	-1.188192084	-2.295704164
O	1.719926121	4.663783333	-0.157423014
H	1.346505099	3.785537270	-0.147186011
H	1.051507077	5.296028382	0.062217004
O	2.069928150	-2.977046214	0.579679042
H	2.045704146	-3.118368227	1.518336112
H	1.586744114	-2.165237153	0.415685028

O	-3.820390275	2.010450146	-1.426294101
H	-4.354294316	2.461956177	-0.788879059
H	-3.078854223	1.633603120	-0.962580068
O	4.667711337	-1.866079136	0.208207016
H	5.401490386	-2.200262157	-0.289088023
H	3.974826285	-2.517510183	0.191625015

Coord_4

C	-0.700330052	-0.329278024	-0.145783009
N	0.617571043	-0.451718035	0.028587002
C	1.300283091	0.697646049	0.044850005
C	-0.614327044	1.946365141	0.018474001
N	-1.347958098	0.844760060	-0.228046014
N	0.730554053	1.911621135	-0.018493004
N	-1.452215102	-1.436519102	-0.220808018
H	-0.998923072	-2.314642168	-0.386378028
H	-2.377556173	-1.327732097	-0.590986041
H	-1.133024080	2.893275207	-0.031470002
N	2.631589188	0.667672047	0.112943009
H	3.141735228	1.526855109	0.190371013
H	3.133183226	-0.194978014	0.144857012
O	4.211176302	3.392049244	0.460429033
H	3.526063255	4.041003292	0.326317024
H	4.967646355	3.684833263	-0.029627004
O	-0.155684010	-4.196521304	-0.714314053
H	0.720916053	-4.054890294	-0.370968026
H	-0.070016003	-4.601230333	-1.566474112
O	-4.094244296	-0.792402057	-1.937711140
H	-4.223997303	0.149998011	-1.956275138
H	-4.877966354	-1.194156086	-2.287271163
O	1.721836123	4.663764336	-0.165603014
H	1.340998095	3.789004275	-0.171984014
H	1.049860076	5.309875384	-0.004745000
O	2.066193148	-2.980765214	0.587785042
H	2.038613145	-3.122429223	1.526264108
H	1.586083114	-2.166593154	0.422799033
O	-3.807934274	2.008678143	-1.457329103
H	-4.334867314	2.470571177	-0.822096060
H	-3.060057223	1.641925120	-0.996605069
O	4.659061337	-1.865505132	0.209124017
H	5.397432391	-2.209852161	-0.274173019
H	3.967386285	-2.518613179	0.202957017

Coord_5

C	-0.691653048	-0.332593023	-0.149243013
N	0.625273043	-0.460565032	0.034056001
C	1.305118094	0.690990047	0.043958003

C	-0.616919044	1.947973141	0.091474008
N	-1.337420094	0.843589060	-0.223459016
N	0.733421051	1.904711139	-0.013407002
N	-1.444330102	-1.435583104	-0.247214016
H	-0.993229072	-2.315450169	-0.410073029
H	-2.371356169	-1.322576096	-0.611700044
H	-1.140787084	2.892327207	0.056397002
N	2.636724192	0.665528049	0.094459007
H	3.144336224	1.525856112	0.177930013
H	3.140229227	-0.196275017	0.126688007
O	4.208072302	3.391769245	0.460466033
H	3.523852252	4.041514292	0.326107025
H	4.969339358	3.690395265	-0.018543001
O	-0.155970009	-4.189497302	-0.720458050
H	0.717472051	-4.048880291	-0.368373026
H	-0.062174003	-4.594316331	-1.571680116
O	-4.095878295	-0.798540058	-1.928464138
H	-4.220374302	0.144180009	-1.957904142
H	-4.879330350	-1.200120088	-2.278837163
O	1.719757123	4.664464337	-0.173293013
H	1.334117097	3.792433275	-0.196612013
H	1.045394074	5.319931382	-0.070255006
O	2.062027148	-2.984361216	0.596044044
H	2.030745147	-3.126422225	1.534316111
H	1.585082117	-2.167852157	0.429938031
O	-3.795479272	2.006906146	-1.488364105
H	-4.315440312	2.479185177	-0.855312061
H	-3.041260217	1.650246120	-1.030630076
O	4.649979337	-1.864708133	0.210796016
H	5.393048390	-2.218780159	-0.257989017
H	3.959516287	-2.519322182	0.214841015

Coord_6

C	-0.682564048	-0.334155022	-0.153566010
N	0.633294048	-0.468969033	0.039088000
C	1.310932095	0.684588050	0.042842005
C	-0.615462044	1.946146141	0.167731011
N	-1.324058094	0.845498061	-0.218968016
N	0.736504053	1.897706139	-0.007881000
N	-1.437059101	-1.431583101	-0.275566020
H	-0.989219073	-2.313616168	-0.436244030
H	-2.365439168	-1.313109094	-0.634679047
H	-1.140896084	2.889699207	0.147800010
N	2.642570193	0.662695046	0.075436005
H	3.148509226	1.523581110	0.165197014
H	3.147464228	-0.198579012	0.107534008
O	4.200551301	3.390751246	0.458931033

H	3.517570251	4.041716289	0.324596023
H	4.966167358	3.694066268	-0.010124002
O	-0.156223009	-4.182812301	-0.726551055
H	0.713893050	-4.042991289	-0.365661024
H	-0.054092006	-4.587972332	-1.576628113
O	-4.097512294	-0.804678059	-1.919218136
H	-4.216751306	0.138363012	-1.959534140
H	-4.880693352	-1.206083085	-2.270403162
O	1.713519124	4.665895338	-0.180626012
H	1.325637095	3.795821274	-0.221054017
H	1.037573072	5.326261384	-0.134038009
O	2.057375150	-2.987823216	0.604500042
H	2.022018146	-3.130290225	1.542537113
H	1.583698112	-2.169009155	0.437102032
O	-3.783023271	2.005135143	-1.519399107
H	-4.296013310	2.487800178	-0.888529062
H	-3.022463217	1.658567120	-1.064655078
O	4.640406336	-1.863660134	0.213230015
H	5.388272385	-2.227042161	-0.240506017
H	3.951156287	-2.519617182	0.227312014

Coord_7

C	-0.672983050	-0.333832023	-0.158882013
N	0.641667044	-0.476910036	0.043550002
C	1.317784094	0.678463051	0.041329002
C	-0.609657044	1.940440139	0.247020019
N	-1.307570095	0.850682062	-0.214654015
N	0.739754053	1.890569136	-0.001988003
N	-1.430400104	-1.424230103	-0.306021023
H	-0.987008070	-2.308897166	-0.465063033
H	-2.359771172	-1.298927096	-0.660086048
H	-1.132560082	2.885228209	0.242218016
N	2.649178193	0.659147050	0.055588006
H	3.154363228	1.519974111	0.151831012
H	3.154899227	-0.201943013	0.087066004
O	4.188362301	3.388993245	0.455949035
H	3.507000253	4.041613290	0.321787023
H	4.957945356	3.695754264	-0.004314001
O	-0.156490011	-4.176573301	-0.732461054
H	0.710128049	-4.037293288	-0.362709025
H	-0.045814002	-4.582363328	-1.581150113
O	-4.099146293	-0.810816060	-1.909972140
H	-4.213128304	0.132545010	-1.961163143
H	-4.882057349	-1.212047087	-2.261969162
O	1.702917121	4.668049338	-0.187729016
H	1.315285097	3.799167273	-0.245291017
H	1.025817072	5.328934386	-0.195824015

O	2.052175148	-2.991131214	0.613206045
H	2.012342145	-3.133968224	1.550984110
H	1.581880113	-2.170057154	0.444291032
O	-3.770568269	2.003363145	-1.550434109
H	-4.276586309	2.496414178	-0.921745068
H	-3.003666216	1.666889120	-1.098681080
O	4.630273332	-1.862333133	0.216426018
H	5.383022386	-2.234630161	-0.221699015
H	3.942229284	-2.519468182	0.240402017

Coord_8

C	-0.662824048	-0.331479026	-0.165344014
N	0.650426045	-0.484365033	0.047283003
C	1.325727098	0.672643049	0.039208002
C	-0.599189045	1.930302140	0.329062025
N	-1.287591092	0.859349064	-0.210637014
N	0.743096051	1.883252134	0.004180998
N	-1.424353100	-1.413201102	-0.338750022
H	-0.986739073	-2.301016167	-0.496713034
H	-2.354306168	-1.279570094	-0.688107047
H	-1.114682082	2.878751207	0.338973022
N	2.656588193	0.654866048	0.034561000
H	3.162001230	1.514986108	0.137411012
H	3.162529227	-0.206416016	0.064882004
O	4.171203300	3.386501243	0.451687030
H	3.491868250	4.041210290	0.317715025
H	4.944437356	3.695384269	-0.000997002
O	-0.156832013	-4.170911300	-0.738021051
H	0.706109049	-4.031864289	-0.359370027
H	-0.037402005	-4.577687327	-1.585038116
O	-4.100781297	-0.816954061	-1.900725138
H	-4.209505303	0.126727008	-1.962792142
H	-4.883420351	-1.218011089	-2.253536161
O	1.687702122	4.670898338	-0.194720013
H	1.302726096	3.802468275	-0.269298022
H	1.009497071	5.328019385	-0.255346020
O	2.046347149	-2.994263218	0.622226046
H	2.001611145	-3.137372225	1.559719112
H	1.579563116	-2.170985156	0.451502030
O	-3.758113273	2.001592142	-1.581469111
H	-4.257159307	2.505028178	-0.954962069
H	-2.984869216	1.675210120	-1.132706082
O	4.619493330	-1.860691133	0.220373018
H	5.377199388	-2.241534162	-0.201544013
H	3.932646286	-2.518840180	0.254143020

Coord_9

C	-0.651994044	-0.326939024	-0.173141012
N	0.659596046	-0.491315035	0.050098004
C	1.334806096	0.667162048	0.036215002
C	-0.583736043	1.915040139	0.413494028
N	-1.263665089	0.871716064	-0.207097014
N	0.746421052	1.875695133	0.010509000
N	-1.418931102	-1.398125102	-0.373953025
H	-0.988597072	-2.289658165	-0.531385040
H	-2.348990169	-1.254510090	-0.718962050
H	-1.085694081	2.870125205	0.437152029
N	2.664817191	0.649840044	0.011905001
H	3.171509227	1.508571109	0.121398008
H	3.170327231	-0.212035016	0.040467004
O	4.148705298	3.383304246	0.446376033
H	3.471824248	4.040520290	0.312463020
H	4.925326352	3.692917265	0.000021998
O	-0.157334011	-4.165984300	-0.743023051
H	0.701751052	-4.026802291	-0.355457026
H	-0.028943000	-4.574184327	-1.588033116
O	-4.102415296	-0.823091062	-1.891479136
H	-4.205882301	0.120910011	-1.964422140
H	-4.884784353	-1.223975086	-2.245102161
O	1.667550121	4.674391337	-0.201705016
H	1.287532094	3.805720276	-0.293045020
H	0.987909073	5.323583382	-0.312326022
O	2.039796147	-2.997188214	0.631633045
H	1.989700143	-3.140397225	1.568823114
H	1.576664113	-2.171782155	0.458734031
O	-3.745657271	1.999820145	-1.612504114
H	-4.237732305	2.513643184	-0.988179070
H	-2.966072216	1.683532120	-1.166731083
O	4.607953334	-1.858690134	0.225043018
H	5.370676384	-2.247731161	-0.180026015
H	3.922290282	-2.517686182	0.268564021

Coord_10

C	-0.650393045	-0.411435031	-0.113881008
N	0.667911050	-0.576125040	0.077044006
C	1.328062097	0.592721044	0.059158005
C	-0.580228042	1.789910130	0.608397046
N	-1.260884088	0.788815055	-0.094298005
N	0.717123053	1.790534131	0.085353004
N	-1.417312100	-1.475636106	-0.340000023
H	-0.989652072	-2.362711169	-0.527389037
H	-2.358813170	-1.326130098	-0.649611048
H	-1.071411079	2.748052200	0.677246049
N	2.654982193	0.593229043	-0.026485004

H	3.156471227	1.454190103	0.090558007
H	3.170841226	-0.263230020	-0.032347002
O	4.079873292	3.338533241	0.435365029
H	3.393767244	3.992053285	0.334504025
H	4.841813350	3.666051265	-0.023349004
O	-0.136873008	-4.235285305	-0.766947054
H	0.728066052	-4.091696297	-0.394011028
H	-0.019987004	-4.627597336	-1.621099116
O	-4.051770292	-0.709232052	-1.926949141
H	-4.147753297	0.238829017	-1.907439138
H	-4.839022348	-1.067751077	-2.313688168
O	1.566507112	4.616540331	-0.112995006
H	1.201576088	3.744312272	-0.226090017
H	0.872186063	5.247531378	-0.237589017
O	2.080192152	-3.070618219	0.576768043
H	2.054780150	-3.232068235	1.511974110
H	1.605238113	-2.246189160	0.431254031
O	-3.668946266	2.075065149	-1.389238099
H	-4.145475300	2.530207183	-0.708835052
H	-2.879247210	1.721269126	-0.990870074
O	4.614780335	-1.885520134	0.110130009
H	5.375323386	-2.264812161	-0.308118020
H	3.940678286	-2.555113185	0.171456011

LIIC path connecting S1-MIN and S₁/S₀

Coord_1

C	-0.650393045	-0.411435031	-0.113881008
N	0.667911050	-0.576125040	0.077044006
C	1.328062097	0.592721044	0.059158005
C	-0.580228042	1.789910130	0.608397046
N	-1.260884088	0.788815055	-0.094298005
N	0.717123053	1.790534131	0.085353004
N	-1.417312100	-1.475636106	-0.340000023
H	-0.989652072	-2.362711169	-0.527389037
H	-2.358813170	-1.326130098	-0.649611048
H	-1.071411079	2.748052200	0.677246049
N	2.654982193	0.593229043	-0.026485004
H	3.156471227	1.454190103	0.090558007
H	3.170841226	-0.263230020	-0.032347002
O	4.079873292	3.338533241	0.435365029
H	3.393767244	3.992053285	0.334504025
H	4.841813350	3.666051265	-0.023349004
O	-0.136873008	-4.235285305	-0.766947054
H	0.728066052	-4.091696297	-0.394011028
H	-0.019987004	-4.627597336	-1.621099116
O	-4.051770292	-0.709232052	-1.926949141
H	-4.147753297	0.238829017	-1.907439138

S21

H	-4.839022348	-1.067751077	-2.313688168
O	1.566507112	4.616540331	-0.112995006
H	1.201576088	3.744312272	-0.226090017
H	0.872186063	5.247531378	-0.237589017
O	2.080192152	-3.070618219	0.576768043
H	2.054780150	-3.232068235	1.511974110
H	1.605238113	-2.246189160	0.431254031
O	-3.668946266	2.075065149	-1.389238099
H	-4.145475300	2.530207183	-0.708835052
H	-2.879247210	1.721269126	-0.990870074
O	4.614780335	-1.885520134	0.110130009
H	5.375323386	-2.264812161	-0.308118020
H	3.940678286	-2.555113185	0.171456011

Coord_2

C	-0.647069045	-0.415356028	-0.117590006
N	0.670139051	-0.582680043	0.075349003
C	1.328324093	0.586835042	0.060233002
C	-0.577081041	1.775931130	0.632940044
N	-1.253005089	0.788470058	-0.098919008
N	0.712806051	1.783626129	0.084875004
N	-1.416524103	-1.475404105	-0.347650026
H	-0.992217073	-2.365035173	-0.531145037
H	-2.358237171	-1.322815093	-0.655389050
H	-1.068867075	2.732347198	0.719709052
N	2.654248193	0.591600045	-0.022975003
H	3.152790228	1.454793106	0.090963008
H	3.173010228	-0.263225019	-0.032268001
O	4.069455295	3.337826239	0.431533029
H	3.380744245	3.988222285	0.327637024
H	4.831799348	3.668587262	-0.024221004
O	-0.137643008	-4.235799305	-0.762955057
H	0.727982050	-4.093169294	-0.391181031
H	-0.022453001	-4.631748334	-1.615667117
O	-4.046830290	-0.703296048	-1.920990139
H	-4.137487296	0.245446019	-1.903568137
H	-4.835216346	-1.058339078	-2.308583168
O	1.552422112	4.608096334	-0.118650006
H	1.188001088	3.735607269	-0.232601019
H	0.860481064	5.239132377	-0.255692017
O	2.083015148	-3.074541222	0.576926039
H	2.057572147	-3.235146231	1.512274111
H	1.607631116	-2.250409163	0.430660030
O	-3.652264260	2.082324148	-1.395183098
H	-4.124301299	2.542466182	-0.714993051
H	-2.860218208	1.730732127	-0.999117074
O	4.612460332	-1.879333137	0.108615006

H	5.376070389	-2.256676161	-0.305839023
H	3.941403285	-2.551928184	0.170962014

Coord_3

C	-0.643631049	-0.419145032	-0.121342010
N	0.672493048	-0.589146044	0.073633003
C	1.328604097	0.581130040	0.061242006
C	-0.573689041	1.761202127	0.657364045
N	-1.244748087	0.788389057	-0.103583007
N	0.708106052	1.776687128	0.084264005
N	-1.415630100	-1.475005105	-0.355306025
H	-0.994736074	-2.367190168	-0.534876038
H	-2.357530169	-1.319300097	-0.661187049
H	-1.066056075	2.715550197	0.762169055
N	2.653515192	0.590266042	-0.019489000
H	3.149028227	1.455713107	0.091313006
H	3.175269228	-0.262845017	-0.032145004
O	4.058269292	3.337856238	0.427267030
H	3.366817241	3.984956288	0.320380025
H	4.820868345	3.672000265	-0.025619000
O	-0.138634009	-4.236156304	-0.758936057
H	0.727676054	-4.094577297	-0.388289029
H	-0.025162002	-4.635784332	-1.610168113
O	-4.042116289	-0.696198051	-1.915745135
H	-4.127211298	0.253200016	-1.899916137
H	-4.831841349	-1.047371075	-2.304105165
O	1.537273111	4.599748330	-0.124625010
H	1.173545082	3.726911268	-0.239358019
H	0.847756061	5.230622376	-0.274114021
O	2.085674153	-3.078517222	0.577164042
H	2.060138149	-3.238225233	1.512660109
H	1.609968116	-2.254632161	0.430083031
O	-3.635039260	2.090326150	-1.400703100
H	-4.102187294	2.555223185	-0.720357051
H	-2.840554203	1.740557123	-1.007494071
O	4.610126332	-1.873614133	0.107258005
H	5.376763389	-2.249067164	-0.303350022
H	3.942038282	-2.549108182	0.170617011

Coord_4

C	-0.640082048	-0.422795032	-0.125126008
N	0.674971048	-0.595522042	0.071907007
C	1.328893096	0.575614040	0.062198007
C	-0.570051043	1.745714125	0.681657049
N	-1.236105088	0.788577058	-0.108275010
N	0.703002053	1.769713128	0.083529004
N	-1.414636104	-1.474435107	-0.362958024

H	-0.997219074	-2.369171169	-0.538571039
H	-2.356700171	-1.315577097	-0.666991049
H	-1.062980079	2.697641193	0.804622056
N	2.652774191	0.589240042	-0.016013999
H	3.145172224	1.456969104	0.091620008
H	3.177612229	-0.262074017	-0.031962004
O	4.046304293	3.338638241	0.422517029
H	3.351968242	3.982263289	0.312702023
H	4.808997344	3.676320267	-0.027604002
O	-0.139851011	-4.236352306	-0.754895053
H	0.727140050	-4.095919296	-0.385337030
H	-0.028117002	-4.639703334	-1.604607117
O	-4.037615292	-0.687908050	-1.911240138
H	-4.116901295	0.262118018	-1.896500139
H	-4.828882349	-1.034799072	-2.300292167
O	1.521030111	4.591488328	-0.130910011
H	1.158182082	3.718215266	-0.246356018
H	0.833987059	5.221996374	-0.292858019
O	2.088162148	-3.082550224	0.577486041
H	2.062466148	-3.241307236	1.513137109
H	1.612245118	-2.258856160	0.429524029
O	-3.617243262	2.099096151	-1.405783101
H	-4.079109292	2.568483187	-0.724908055
H	-2.820237205	1.750755125	-1.015990076
O	4.607782331	-1.868371135	0.106066007
H	5.377403386	-2.241997160	-0.300643021
H	3.942579281	-2.546661182	0.170429010

Coord_5

C	-0.636427047	-0.426304033	-0.128932010
N	0.677570049	-0.601803043	0.070178005
C	1.329181096	0.570294041	0.063115002
C	-0.566169041	1.729455122	0.705809053
N	-1.227069090	0.789038056	-0.112980009
N	0.697477051	1.762701127	0.082679008
N	-1.413547099	-1.473686104	-0.370596025
H	-0.999672070	-2.370971171	-0.542222040
H	-2.355750171	-1.311636097	-0.672793049
H	-1.059641076	2.678597194	0.847064061
N	2.652014192	0.588540041	-0.012535003
H	3.141203225	1.458576104	0.091902006
H	3.180035231	-0.260889019	-0.031704004
O	4.033548290	3.340190238	0.417230030
H	3.336176238	3.980149289	0.304571024
H	4.796162346	3.681577267	-0.030240003
O	-0.141297009	-4.236381305	-0.750840052
H	0.726369055	-4.097191295	-0.382326027

H	-0.031320001	-4.643499334	-1.598989117
O	-4.033314288	-0.678395047	-1.907505137
H	-4.106532295	0.272229018	-1.893332135
H	-4.826324348	-1.020568073	-2.297179166
O	1.503663106	4.583307333	-0.137495008
H	1.141883084	3.709506268	-0.253588019
H	0.819150056	5.213243375	-0.311925022
O	2.090469149	-3.086640225	0.577897043
H	2.064545148	-3.244391233	1.513709108
H	1.614454116	-2.263082164	0.428986030
O	-3.598849257	2.108655151	-1.410407099
H	-4.055036294	2.582254184	-0.728622053
H	-2.799249199	1.761334125	-1.024590074
O	4.605427333	-1.863614133	0.105045007
H	5.377992387	-2.235480162	-0.297708024
H	3.943026283	-2.544594184	0.170404012

Coord_6

C	-0.632666046	-0.429666034	-0.132748008
N	0.680285051	-0.607985045	0.068459005
C	1.329460094	0.565176040	0.064005004
C	-0.562044040	1.712412122	0.729806050
N	-1.217631087	0.789780058	-0.117686009
N	0.691510048	1.755645125	0.081724007
N	-1.412368103	-1.472752106	-0.378209028
H	-1.002103073	-2.372585172	-0.545816037
H	-2.354684170	-1.307468096	-0.678581047
H	-1.056042078	2.658394191	0.889488063
N	2.651225188	0.588182042	-0.009037998
H	3.137105224	1.460556105	0.092173009
H	3.182531227	-0.259271018	-0.031357001
O	4.019987287	3.342529239	0.411352029
H	3.319419237	3.978623285	0.295952023
H	4.782334346	3.687804265	-0.033592002
O	-0.142978009	-4.236236305	-0.746776056
H	0.725356051	-4.098389294	-0.379259027
H	-0.034776005	-4.647164337	-1.593319115
O	-4.029203290	-0.667624046	-1.904571135
H	-4.096079292	0.283566021	-1.890427137
H	-4.824156346	-1.004618072	-2.294808166
O	1.485137108	4.575192331	-0.144371010
H	1.124617084	3.700772267	-0.261048021
H	0.803216058	5.204352377	-0.331317024
O	2.092588150	-3.090789223	0.578402042
H	2.066362146	-3.247476236	1.514383110
H	1.616591119	-2.267311164	0.428469029
O	-3.579825256	2.119028152	-1.414558103

H	-4.029934290	2.596537186	-0.731472054
H	-2.777568199	1.772301127	-1.033284075
O	4.603065329	-1.859351134	0.104203007
H	5.378529385	-2.229530162	-0.294535019
H	3.943376286	-2.542916184	0.170551012

Coord_7

C	-0.628802047	-0.432877033	-0.136561010
N	0.683117049	-0.614065043	0.066758007
C	1.329720094	0.560268042	0.064882004
C	-0.557673042	1.694572123	0.753635055
N	-1.207781088	0.790805058	-0.122376007
N	0.685080047	1.748539127	0.080673008
N	-1.411103100	-1.471627107	-0.385785026
H	-1.004518074	-2.374005172	-0.549342040
H	-2.353505168	-1.303064092	-0.684342052
H	-1.052181074	2.637004190	0.931886067
N	2.650394190	0.588183042	-0.005504999
H	3.132859227	1.462926105	0.092450007
H	3.185097229	-0.257197018	-0.030903004
O	4.005606287	3.345677240	0.404822030
H	3.301673236	3.977696288	0.286810021
H	4.767481341	3.695038266	-0.037732005
O	-0.144898013	-4.235908305	-0.742712054
H	0.724095053	-4.099508297	-0.376138030
H	-0.038486003	-4.650690335	-1.587605112
O	-4.025276292	-0.655554047	-1.902472137
H	-4.085520296	0.296162022	-1.887802137
H	-4.822370346	-0.986879072	-2.293220163
O	1.465418107	4.567132331	-0.151526011
H	1.106353081	3.692000265	-0.268730019
H	0.786158056	5.195310373	-0.351038026
O	2.094509153	-3.094997225	0.579007039
H	2.067904148	-3.250563234	1.515163107
H	1.618650116	-2.271541163	0.427976032
O	-3.560137258	2.130236153	-1.418214104
H	-4.003767290	2.611334188	-0.733429052
H	-2.755174201	1.783663129	-1.042055077
O	4.600696330	-1.855596135	0.103549007
H	5.379017387	-2.224163162	-0.291113020
H	3.943626285	-2.541637184	0.170878012

Coord_8

C	-0.624835043	-0.435931032	-0.140361011
N	0.686063047	-0.620038046	0.065087002
C	1.329953096	0.555579040	0.065760005
C	-0.553058039	1.675920122	0.777281055

N	-1.197510085	0.792117058	-0.127036010
N	0.678168051	1.741378126	0.079538008
N	-1.409753100	-1.470303106	-0.393313028
H	-1.006922073	-2.375225169	-0.552790037
H	-2.352215171	-1.298416096	-0.690065051
H	-1.048060074	2.614397188	0.974251072
N	2.649511189	0.588563044	-0.001918998
H	3.128447228	1.465709106	0.092752008
H	3.187727229	-0.254642018	-0.030324005
O	3.990388287	3.349658241	0.397581027
H	3.282910235	3.977378284	0.277106021
H	4.751571341	3.703319265	-0.042733005
O	-0.147061009	-4.235388304	-0.738656053
H	0.722579050	-4.100544294	-0.372967025
H	-0.042454002	-4.654069338	-1.581854114
O	-4.021530288	-0.642142045	-1.901246139
H	-4.074834292	0.310057021	-1.885474138
H	-4.820961348	-0.967277071	-2.292461164
O	1.444466106	4.559111327	-0.158951013
H	1.087056077	3.683172265	-0.276628021
H	0.767945056	5.186104371	-0.371091028
O	2.096224153	-3.099266225	0.579716042
H	2.069157150	-3.253650237	1.516054109
H	1.620628117	-2.275773163	0.427509033
O	-3.539748255	2.142302156	-1.421354104
H	-3.976491288	2.626643191	-0.734462053
H	-2.732042196	1.795426131	-1.050892077
O	4.598325330	-1.852361131	0.103092010
H	5.379458388	-2.219399159	-0.287429021
H	3.943776286	-2.540768185	0.171395013

Coord_9

C	-0.620766046	-0.438826034	-0.144134013
N	0.689124052	-0.625900044	0.063457004
C	1.330150093	0.551118038	0.066655002
C	-0.548198038	1.656442119	0.800727057
N	-1.186805084	0.793721057	-0.131648007
N	0.670751049	1.734154126	0.078327007
N	-1.408321104	-1.468777107	-0.400780031
H	-1.009320072	-2.376240173	-0.556146043
H	-2.350815169	-1.293517094	-0.695738048
H	-1.043679074	2.590544184	1.016571075
N	2.648564189	0.589342040	0.001736998
H	3.123849222	1.468927107	0.093097005
H	3.190418228	-0.251581019	-0.029601001
O	3.974316285	3.354499244	0.389561029
H	3.263100236	3.977681286	0.266799019

H	4.734567342	3.712691270	-0.048674004
O	-0.149473009	-4.234666305	-0.734619055
H	0.720801052	-4.101490294	-0.369751024
H	-0.046684001	-4.657289334	-1.576075112
O	-4.017965290	-0.627337046	-1.900934136
H	-4.063998292	0.325291023	-1.883461137
H	-4.819926346	-0.945727069	-2.292578165
O	1.422240101	4.551116327	-0.166635011
H	1.066691077	3.674273266	-0.284736022
H	0.748549053	5.176717370	-0.391479026
O	2.097723153	-3.103598223	0.580536044
H	2.070107150	-3.256737234	1.517062107
H	1.622519116	-2.280007163	0.427069033
O	-3.518619255	2.155248155	-1.423954100
H	-3.948063283	2.642462188	-0.734536054
H	-2.708150193	1.807593128	-1.059779075
O	4.595954330	-1.849661131	0.102842005
H	5.379853387	-2.215256162	-0.283470018
H	3.943822282	-2.540322184	0.172112011

Coord_10

C	-0.615783043	-0.442862031	-0.147472010
N	0.693131051	-0.632841045	0.062245003
C	1.331031094	0.545752038	0.067935003
C	-0.542433039	1.634818116	0.824357060
N	-1.174951085	0.794264057	-0.135785009
N	0.663439048	1.725661122	0.077424008
N	-1.405914099	-1.468414107	-0.407765028
H	-1.010745072	-2.378380171	-0.559002039
H	-2.348434168	-1.289810091	-0.700915052
H	-1.038455073	2.564064187	1.059250078
N	2.648268188	0.589514044	0.005805000
H	3.119696223	1.471618106	0.093822004
H	3.193960228	-0.248964015	-0.028405002
O	3.957864286	3.359311243	0.380991030
H	3.242652235	3.977643286	0.256165017
H	4.716882338	3.722351268	-0.055357004
O	-0.151016011	-4.234992305	-0.730240055
H	0.719874050	-4.103528293	-0.366141025
H	-0.050040006	-4.661589338	-1.569909113
O	-4.013801290	-0.612674042	-1.901106135
H	-4.052288293	0.340314026	-1.881303137
H	-4.818463346	-0.923795069	-2.293128166
O	1.399079102	4.541993327	-0.174201012
H	1.045676078	3.664118265	-0.292677019
H	0.728260054	5.165940374	-0.411824029
O	2.100053153	-3.109070223	0.581794041

H	2.071832151	-3.260906236	1.518514111
H	1.625302117	-2.285357166	0.426995033
O	-3.496148251	2.167546155	-1.425514104
H	-3.917898280	2.657195191	-0.733131051
H	-2.682875195	1.818687133	-1.068251076
O	4.594523329	-1.848372135	0.103080008
H	5.381163386	-2.212549161	-0.278971022
H	3.944761286	-2.541226183	0.173322012

LIIC path connecting S₁/S₀ and S₀-MIN

Coord_1

C	-0.615783043	-0.442862031	-0.147472010
N	0.693131051	-0.632841045	0.062245003
C	1.331031094	0.545752038	0.067935003
C	-0.542433039	1.634818116	0.824357060
N	-1.174951085	0.794264057	-0.135785009
N	0.663439048	1.725661122	0.077424008
N	-1.405914099	-1.468414107	-0.407765028
H	-1.010745072	-2.378380171	-0.559002039
H	-2.348434168	-1.289810091	-0.700915052
H	-1.038455073	2.564064187	1.059250078
N	2.648268188	0.589514044	0.005805000
H	3.119696223	1.471618106	0.093822004
H	3.193960228	-0.248964015	-0.028405002
O	3.957864286	3.359311243	0.380991030
H	3.242652235	3.977643286	0.256165017
H	4.716882338	3.722351268	-0.055357004
O	-0.151016011	-4.234992305	-0.730240055
H	0.719874050	-4.103528293	-0.366141025
H	-0.050040006	-4.661589338	-1.569909113
O	-4.013801290	-0.612674042	-1.901106135
H	-4.052288293	0.340314026	-1.881303137
H	-4.818463346	-0.923795069	-2.293128166
O	1.399079102	4.541993327	-0.174201012
H	1.045676078	3.664118265	-0.292677019
H	0.728260054	5.165940374	-0.411824029
O	2.100053153	-3.109070223	0.581794041
H	2.071832151	-3.260906236	1.518514111
H	1.625302117	-2.285357166	0.426995033
O	-3.496148251	2.167546155	-1.425514104
H	-3.917898280	2.657195191	-0.733131051
H	-2.682875195	1.818687133	-1.068251076
O	4.594523329	-1.848372135	0.103080008
H	5.381163386	-2.212549161	-0.278971022
H	3.944761286	-2.541226183	0.173322012

Coord_2

C	-0.627850047	-0.427978032	-0.146680012
N	0.682367051	-0.609365044	0.056416005
C	1.326608093	0.565132038	0.065564003
C	-0.547157041	1.667097118	0.712749054
N	-1.196044085	0.802234059	-0.147656010
N	0.670122048	1.748724127	0.065323005
N	-1.414072102	-1.463290105	-0.379417029
H	-1.012320073	-2.369372172	-0.533480037
H	-2.353925171	-1.293130091	-0.683225048
H	-1.041842078	2.600120187	0.911440066
N	2.645126193	0.598624042	0.023642999
H	3.122210223	1.477437108	0.108670009
H	3.184982228	-0.242999018	-0.003587002
O	3.984331287	3.362712244	0.388544029
H	3.272351234	3.984444287	0.263066018
H	4.741075343	3.715343268	-0.058115002
O	-0.151344011	-4.233070307	-0.726587055
H	0.721129052	-4.100020298	-0.367660028
H	-0.054645002	-4.657304336	-1.567849110
O	-4.022181288	-0.630502045	-1.908330140
H	-4.072567291	0.321202023	-1.889167134
H	-4.824607348	-0.951757070	-2.295358166
O	1.433030104	4.555886331	-0.170414013
H	1.079945078	3.676959264	-0.271068019
H	0.763812055	5.176158374	-0.344035026
O	2.097453151	-3.093400221	0.579692044
H	2.070321149	-3.244022232	1.516657107
H	1.621102117	-2.271544164	0.424067031
O	-3.534942256	2.150584156	-1.418789103
H	-3.970702285	2.633685190	-0.732027055
H	-2.731045194	1.796378131	-1.049036073
O	4.604486329	-1.850251132	0.114687008
H	5.384271387	-2.208680161	-0.283117020
H	3.949670283	-2.538076181	0.172896013

Coord_3

C	-0.639918045	-0.413092027	-0.145888008
N	0.671602046	-0.585890043	0.050588006
C	1.322184097	0.584511044	0.063194003
C	-0.551881038	1.699377121	0.601141042
N	-1.217138090	0.810204061	-0.159528012
N	0.676804049	1.771787127	0.053223002
N	-1.422229104	-1.458166103	-0.351069025
H	-1.013895073	-2.360363167	-0.507958035
H	-2.359415168	-1.296450091	-0.665534050
H	-1.045230077	2.636176192	0.763629055
N	2.641983192	0.607733045	0.041481003

H	3.124723227	1.483256105	0.123517008
H	3.176004228	-0.237034016	0.021231004
O	4.010796288	3.366111245	0.396097029
H	3.302049238	3.991244289	0.269967018
H	4.765266343	3.708334268	-0.060872005
O	-0.151671010	-4.231147303	-0.722934054
H	0.722385054	-4.096511297	-0.369179026
H	-0.059250003	-4.653018333	-1.565789113
O	-4.030561291	-0.648331048	-1.915554140
H	-4.092845294	0.302090019	-1.897031137
H	-4.830749349	-0.979720071	-2.297588167
O	1.466982106	4.569779329	-0.166627009
H	1.114214078	3.689799263	-0.249459018
H	0.799364055	5.186375374	-0.276245018
O	2.094851150	-3.077730224	0.577590040
H	2.068810147	-3.227137234	1.514800107
H	1.616901116	-2.257730161	0.421139030
O	-3.573736256	2.133621152	-1.412063101
H	-4.023506289	2.610175189	-0.730923054
H	-2.779214199	1.774068130	-1.029820075
O	4.614447334	-1.852129135	0.126294008
H	5.387377388	-2.204810160	-0.287264023
H	3.954579286	-2.534925184	0.172471010

Coord_4

C	-0.651985048	-0.398207028	-0.145096010
N	0.660837046	-0.562414041	0.044759002
C	1.317761096	0.603890044	0.060823003
C	-0.556605040	1.731656124	0.489533036
N	-1.238231090	0.818174058	-0.171399013
N	0.683487049	1.794849132	0.041122004
N	-1.430386102	-1.453042106	-0.322722021
H	-1.015470074	-2.351355168	-0.482437033
H	-2.364905170	-1.299770096	-0.647843046
H	-1.048617076	2.672232192	0.615819043
N	2.638841192	0.616842043	0.059319002
H	3.127236227	1.489075108	0.138364012
H	3.167025228	-0.231069019	0.046050004
O	4.037261289	3.369511241	0.403650029
H	3.331747242	3.998044286	0.276868019
H	4.789457347	3.701325267	-0.063630003
O	-0.151998010	-4.229223304	-0.719281054
H	0.723640051	-4.093002296	-0.370697029
H	-0.063855004	-4.648731336	-1.563729111
O	-4.038940289	-0.666159050	-1.922778139
H	-4.113123298	0.282977021	-1.904895139
H	-4.836892346	-1.007682072	-2.299817167

O	1.500933107	4.583671332	-0.162840011
H	1.148483083	3.702639267	-0.227850018
H	0.834916062	5.196591373	-0.208456016
O	2.092250148	-3.062060222	0.575488042
H	2.067298150	-3.210252231	1.512943108
H	1.612700115	-2.243916163	0.418210029
O	-3.612530262	2.116658153	-1.405338100
H	-4.076310294	2.586665188	-0.729819052
H	-2.827383204	1.751758128	-1.010605073
O	4.624408334	-1.854008132	0.137901009
H	5.390484389	-2.200941160	-0.291410021
H	3.959487283	-2.531775183	0.172045012

Coord_5

C	-0.664053047	-0.383323029	-0.144304011
N	0.650073046	-0.538938040	0.038930004
C	1.313337095	0.623269044	0.058452003
C	-0.561329043	1.763936126	0.377925030
N	-1.259324090	0.826144060	-0.183270015
N	0.690170050	1.817912132	0.029022001
N	-1.438543104	-1.447918104	-0.294374022
H	-1.017044075	-2.342346169	-0.456915032
H	-2.370395172	-1.303089096	-0.630152047
H	-1.052005075	2.708287197	0.468009032
N	2.635698191	0.625951046	0.077157006
H	3.129748226	1.494894110	0.153211011
H	3.158047228	-0.225105017	0.070868005
O	4.063726295	3.372910241	0.411203029
H	3.361445240	4.004844287	0.283769019
H	4.813648346	3.694316267	-0.066387006
O	-0.152325010	-4.227300306	-0.715628053
H	0.724895053	-4.089493295	-0.372216027
H	-0.068460005	-4.644445334	-1.561669114
O	-4.047320292	-0.683988048	-1.930002139
H	-4.133401296	0.263865017	-1.912759136
H	-4.843035348	-1.035645073	-2.302047168
O	1.534884109	4.597563331	-0.159053012
H	1.182751083	3.715479267	-0.206241017
H	0.870467062	5.206808373	-0.140666013
O	2.089649152	-3.046389220	0.573385039
H	2.065787148	-3.193367232	1.511086108
H	1.608500115	-2.230102161	0.415282028
O	-3.651324262	2.099695154	-1.398612098
H	-4.129114299	2.563155182	-0.728714051
H	-2.875552209	1.729448126	-0.991390070
O	4.634369333	-1.855886134	0.149508009
H	5.393590389	-2.197071160	-0.295556019

H 3.964396286 -2.528624181 0.171620014

Coord_6

C -0.676120050 -0.368437024 -0.143512013
N 0.639308046 -0.515462038 0.033102000
C 1.308914094 0.642648044 0.056081004
C -0.566053040 1.796215129 0.266317018
N -1.280417095 0.834114062 -0.195142016
N 0.696852050 1.840974131 0.016921003
N -1.446701102 -1.442794102 -0.266026018
H -1.018619076 -2.333337170 -0.431394030
H -2.375885169 -1.306409096 -0.612461043
H -1.055392074 2.744343196 0.320198025
N 2.632556191 0.635060044 0.094995005
H 3.132261225 1.500713107 0.168059011
H 3.149069228 -0.219140014 0.095687005
O 4.090191296 3.376310242 0.418756029
H 3.391143244 4.011644289 0.290670020
H 4.837838351 3.687307267 -0.069145003
O -0.152652010 -4.225377302 -0.711976053
H 0.726150055 -4.085985295 -0.373735025
H -0.073065006 -4.640159332 -1.559609111
O -4.055699290 -0.701816051 -1.937226139
H -4.153678299 0.244752018 -1.920622139
H -4.849177349 -1.063607074 -2.304276168
O 1.568836111 4.611456334 -0.155266013
H 1.217020089 3.728318271 -0.184631011
H 0.906019063 5.217024378 -0.072877005
O 2.087048151 -3.030719218 0.571283041
H 2.064275151 -3.176483229 1.509229109
H 1.604299114 -2.216288158 0.412354032
O -3.690117267 2.082732149 -1.391887102
H -4.181917303 2.539645181 -0.727610055
H -2.923721208 1.707138125 -0.972174072
O 4.644330333 -1.857765132 0.161115009
H 5.396696390 -2.193202160 -0.299703022
H 3.969304288 -2.525473184 0.171194010

Coord_7

C -0.688188048 -0.353552025 -0.142720009
N 0.628543047 -0.491986037 0.027273002
C 1.304491093 0.662027049 0.053711004
C -0.570777042 1.828494131 0.154709012
N -1.301511095 0.842084059 -0.207013013
N 0.703535051 1.864037136 0.004821001
N -1.454858105 -1.437670105 -0.237678019
H -1.020194071 -2.324329165 -0.405872028

H	-2.381375171	-1.309729096	-0.594770044
H	-1.058780078	2.780399202	0.172388014
N	2.629413190	0.644169047	0.112833009
H	3.134774224	1.506533110	0.182906015
H	3.140090228	-0.213175017	0.120505010
O	4.116656297	3.379709243	0.426308028
H	3.420841248	4.018444291	0.297570020
H	4.862029350	3.680298267	-0.071902006
O	-0.152979010	-4.223454304	-0.708323052
H	0.727405051	-4.082476294	-0.375254029
H	-0.077669006	-4.635872334	-1.557549114
O	-4.064078293	-0.719645053	-1.944449138
H	-4.173956302	0.225640015	-1.928486141
H	-4.855320351	-1.091569081	-2.306506164
O	1.602787117	4.625348332	-0.151478009
H	1.251289089	3.741158270	-0.163022011
H	0.941571069	5.227241378	-0.005087002
O	2.084447149	-3.015048216	0.569181043
H	2.062764149	-3.159598225	1.507372110
H	1.600098114	-2.202474160	0.409425030
O	-3.728911267	2.065769150	-1.385161101
H	-4.234721303	2.516135180	-0.726506053
H	-2.971890213	1.684828123	-0.952959070
O	4.654292333	-1.859643134	0.172722015
H	5.399803390	-2.189333160	-0.303849020
H	3.974213286	-2.522323183	0.170768012

Coord_8

C	-0.700255052	-0.338668026	-0.141928011
N	0.617779047	-0.468511036	0.021444003
C	1.300067092	0.681407049	0.051340004
C	-0.575501039	1.860774134	0.043101005
N	-1.322604095	0.850054061	-0.218884014
N	0.710218052	1.887099136	-0.007280003
N	-1.463015107	-1.432546103	-0.209330015
H	-1.021768072	-2.315320166	-0.380350027
H	-2.386865174	-1.313049095	-0.577079040
H	-1.062167077	2.816455202	0.024578002
N	2.626271190	0.653278045	0.130670008
H	3.137287224	1.512352107	0.197753014
H	3.131112228	-0.207210015	0.145324011
O	4.143121298	3.383109244	0.433861033
H	3.450539247	4.025244287	0.304471020
H	4.886220349	3.673289266	-0.074660004
O	-0.153306009	-4.221530306	-0.704670052
H	0.728661054	-4.078967293	-0.376773027
H	-0.082274007	-4.631586332	-1.555489112

O	-4.072458291	-0.737473051	-1.951673138
H	-4.194234301	0.206527016	-1.936350139
H	-4.861463353	-1.119532082	-2.308735164
O	1.636739119	4.639240336	-0.147691010
H	1.285557094	3.753998269	-0.141413010
H	0.977123070	5.237458377	0.062702006
O	2.081846148	-2.999378214	0.567079040
H	2.061253147	-3.142713227	1.505514110
H	1.595898113	-2.188661158	0.406497029
O	-3.767705272	2.048806146	-1.378436099
H	-4.287525307	2.492625179	-0.725402052
H	-3.020059217	1.662519121	-0.933744067
O	4.664253338	-1.861522131	0.184329015
H	5.402909391	-2.185463160	-0.307995023
H	3.979121288	-2.519172181	0.170343014

Coord_9

C	-0.712323050	-0.323782021	-0.141136012
N	0.607014042	-0.445035034	0.015615999
C	1.295644096	0.700786049	0.048969004
C	-0.580225041	1.893053137	-0.068507006
N	-1.343697094	0.858024063	-0.230756016
N	0.716900052	1.910161135	-0.019380000
N	-1.471172105	-1.427422101	-0.180982011
H	-1.023343073	-2.306311167	-0.354829025
H	-2.392355171	-1.316368095	-0.559388042
H	-1.065554076	2.852510207	-0.123232009
N	2.623128189	0.662387048	0.148508012
H	3.139800228	1.518171109	0.212600013
H	3.122133222	-0.201245012	0.170142011
O	4.169587299	3.386508244	0.441414033
H	3.480237251	4.032044289	0.311372021
H	4.910411354	3.666280266	-0.077417007
O	-0.153633009	-4.219607302	-0.701017051
H	0.729916050	-4.075458292	-0.378292030
H	-0.086879008	-4.627300335	-1.553428110
O	-4.080837294	-0.755302054	-1.958897143
H	-4.214512304	0.187415013	-1.944213141
H	-4.867605349	-1.147494083	-2.310965164
O	1.670690121	4.653133334	-0.143904011
H	1.319826094	3.766838273	-0.119804009
H	1.012675071	5.247674377	0.130492009
O	2.079245152	-2.983708217	0.564976042
H	2.059741150	-3.125828224	1.503657111
H	1.591697113	-2.174847155	0.403569028
O	-3.806498272	2.031843147	-1.371711098
H	-4.340329312	2.469115178	-0.724297051

H	-3.068228222	1.640209120	-0.914528064
O	4.674214338	-1.863400134	0.195936015
H	5.406015392	-2.181594160	-0.312142021
H	3.984030286	-2.516021179	0.169917010

Coord_10

C	-0.724575054	-0.309980020	-0.139502008
N	0.596051045	-0.422714031	0.010687999
C	1.291079095	0.718973051	0.047564002
C	-0.585017043	1.924243140	-0.179204013
N	-1.364910096	0.864947061	-0.241782016
N	0.723508053	1.932063141	-0.030508000
N	-1.479571105	-1.423341101	-0.151859011
H	-1.025196072	-2.298364163	-0.328535022
H	-2.398063173	-1.320673095	-0.540962037
H	-1.068956077	2.887504206	-0.270127020
N	2.619836188	0.670232048	0.167373012
H	3.142204227	1.522697109	0.228523015
H	3.112959226	-0.196570012	0.195986012
O	4.196028301	3.388554245	0.450144034
H	3.509951252	4.037529291	0.319436021
H	4.934617355	3.657894262	-0.078955008
O	-0.154320013	-4.218779304	-0.696605052
H	0.730803052	-4.073099294	-0.379006028
H	-0.091825006	-4.624088335	-1.550617109
O	-4.089339294	-0.773988054	-1.965449140
H	-4.234864308	0.167451012	-1.951386139
H	-4.873874353	-1.176264085	-2.312571165
O	1.704712122	4.665816337	-0.139021012
H	1.354118097	3.778486274	-0.097140009
H	1.048312074	5.256706380	0.199363015
O	2.076288152	-2.969283216	0.563773042
H	2.057823147	-3.110214224	1.502694109
H	1.587190115	-2.162249154	0.401539030
O	-3.845299278	2.013992146	-1.364224097
H	-4.393147319	2.444727176	-0.722446052
H	-3.116447223	1.616960114	-0.894529064
O	4.683892339	-1.866649134	0.208595015
H	5.408847389	-2.179117155	-0.315210022
H	3.988624285	-2.514204180	0.170493014

LIIC path connecting S1-MIN and T1-MIN

Coord_1

C	-0.650393045	-0.411435031	-0.113881008
N	0.667911050	-0.576125040	0.077044006
C	1.328062097	0.592721044	0.059158005
C	-0.580228042	1.789910130	0.608397046

N	-1.260884088	0.788815055	-0.094298005
N	0.717123053	1.790534131	0.085353004
N	-1.417312100	-1.475636106	-0.340000023
H	-0.989652072	-2.362711169	-0.527389037
H	-2.358813170	-1.326130098	-0.649611048
H	-1.071411079	2.748052200	0.677246049
N	2.654982193	0.593229043	-0.026485004
H	3.156471227	1.454190103	0.090558007
H	3.170841226	-0.263230020	-0.032347002
O	4.079873292	3.338533241	0.435365029
H	3.393767244	3.992053285	0.334504025
H	4.841813350	3.666051265	-0.023349004
O	-0.136873008	-4.235285305	-0.766947054
H	0.728066052	-4.091696297	-0.394011028
H	-0.019987004	-4.627597336	-1.621099116
O	-4.051770292	-0.709232052	-1.926949141
H	-4.147753297	0.238829017	-1.907439138
H	-4.839022348	-1.067751077	-2.313688168
O	1.566507112	4.616540331	-0.112995006
H	1.201576088	3.744312272	-0.226090017
H	0.872186063	5.247531378	-0.237589017
O	2.080192152	-3.070618219	0.576768043
H	2.054780150	-3.232068235	1.511974110
H	1.605238113	-2.246189160	0.431254031
O	-3.668946266	2.075065149	-1.389238099
H	-4.145475300	2.530207183	-0.708835052
H	-2.879247210	1.721269126	-0.990870074
O	4.614780335	-1.885520134	0.110130009
H	5.375323386	-2.264812161	-0.308118020
H	3.940678286	-2.555113185	0.171456011

Coord_2

C	-0.659612048	-0.402558029	-0.115775007
N	0.661201046	-0.565921042	0.078234004
C	1.325453095	0.603395041	0.064644007
C	-0.589157040	1.809172129	0.576993044
N	-1.273372089	0.792855059	-0.099724008
N	0.722034051	1.802197128	0.089236006
N	-1.420673101	-1.472284107	-0.339421024
H	-0.988318069	-2.357143172	-0.526171035
H	-2.361645168	-1.327492094	-0.653289047
H	-1.078528079	2.769879200	0.617353043
N	2.653490189	0.595287045	-0.011907001
H	3.159105228	1.454011104	0.104232006
H	3.164939227	-0.263698019	-0.017133002
O	4.102834293	3.322550242	0.418334031
H	3.417793246	3.979049288	0.329222021

H	4.860299348	3.649826261	-0.047872004
O	-0.134124011	-4.232623305	-0.772523053
H	0.731542053	-4.094766292	-0.399366027
H	-0.020244004	-4.628079332	-1.625602118
O	-4.046273294	-0.730823055	-1.921432140
H	-4.150809301	0.216397013	-1.902893135
H	-4.832166349	-1.096901081	-2.303805163
O	1.593377113	4.618439331	-0.096792006
H	1.222853088	3.746679271	-0.201712017
H	0.893653064	5.250683379	-0.173515013
O	2.080514151	-3.070247218	0.578415044
H	2.055917145	-3.232714233	1.513508110
H	1.604763113	-2.246787162	0.434015029
O	-3.690657266	2.055679148	-1.388771100
H	-4.172675302	2.514936181	-0.714892052
H	-2.902004208	1.708297123	-0.982712071
O	4.615566332	-1.883031133	0.114866008
H	5.375878387	-2.254288164	-0.310839023
H	3.944468285	-2.555929182	0.171429012

Coord_3

C	-0.668514048	-0.393682028	-0.117803010
N	0.654890046	-0.555604038	0.079200006
C	1.323092096	0.614293044	0.069572007
C	-0.597209043	1.827553133	0.544953039
N	-1.285262093	0.797004057	-0.105463010
N	0.726649053	1.813776130	0.092440005
N	-1.423609103	-1.469036107	-0.338532022
H	-0.986503070	-2.351666171	-0.524433037
H	-2.364068170	-1.329157097	-0.656566046
H	-1.084369079	2.790173201	0.556849039
N	2.652125192	0.597656045	0.002004000
H	3.161832227	1.454164105	0.117023008
H	3.159243227	-0.263779020	-0.002464998
O	4.123583296	3.309848236	0.401700027
H	3.439112247	3.968502288	0.323649023
H	4.876407350	3.637522261	-0.071663003
O	-0.131940007	-4.229677307	-0.777585057
H	0.734459053	-4.097703295	-0.404272029
H	-0.021205000	-4.628516331	-1.629485115
O	-4.042713291	-0.749259056	-1.918378136
H	-4.154945298	0.197119012	-1.899384139
H	-4.827867350	-1.121691083	-2.296077165
O	1.617389118	4.620594331	-0.082093008
H	1.242529088	3.748876272	-0.178517014
H	0.914201064	5.252643378	-0.110108006
O	2.080632152	-3.070015222	0.580246039

H	2.056875147	-3.233248231	1.515268112
H	1.604336115	-2.247405161	0.436789029
O	-3.711274265	2.038135149	-1.387201100
H	-4.197789303	2.500726179	-0.718760052
H	-2.923676212	1.695752125	-0.974795071
O	4.616732332	-1.882011134	0.119384007
H	5.376516385	-2.245921163	-0.313498022
H	3.948224285	-2.557687183	0.171380011

Coord_4

C	-0.677096049	-0.384815028	-0.119993010
N	0.648986047	-0.545204038	0.079849005
C	1.321036095	0.625356045	0.073735008
C	-0.604283043	1.845082134	0.512139038
N	-1.296525091	0.801273057	-0.111571006
N	0.731085051	1.825249132	0.094713007
N	-1.426155102	-1.465890106	-0.337254022
H	-0.984274070	-2.346296170	-0.522075039
H	-2.366131168	-1.331120096	-0.659312047
H	-1.088815078	2.808977202	0.495562037
N	2.650942190	0.600212045	0.014968001
H	3.164759228	1.454507107	0.128570010
H	3.153765226	-0.263623019	0.011401002
O	4.141950297	3.300212236	0.386758030
H	3.457659248	3.960282287	0.318418021
H	4.890276350	3.628574260	-0.093189008
O	-0.130343008	-4.226527305	-0.781961056
H	0.736831053	-4.100550295	-0.408660030
H	-0.022982004	-4.628972334	-1.632590116
O	-4.040936292	-0.764905054	-1.917222138
H	-4.160065299	0.180649011	-1.896612134
H	-4.825935350	-1.142658080	-2.289892162
O	1.638701118	4.623006331	-0.069536007
H	1.260829091	3.750875271	-0.156933011
H	0.933979069	5.253253376	-0.047817001
O	2.080644148	-3.069904222	0.582167043
H	2.057856146	-3.233673235	1.517159111
H	1.604003114	-2.248042164	0.439552033
O	-3.730835271	2.022317147	-1.384701097
H	-4.220915306	2.487674180	-0.720740053
H	-2.944260212	1.683685121	-0.967123070
O	4.618227332	-1.882219137	0.123392011
H	5.377202389	-2.239340161	-0.316503024
H	3.951972283	-2.560242183	0.171054011

Coord_5

C	-0.685347049	-0.375978028	-0.122371011
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N	0.643509047	-0.534759037	0.080077006
C	1.319349094	0.636523045	0.076894005
C	-0.610281044	1.861774136	0.478388034
N	-1.307129094	0.805658058	-0.118105006
N	0.735456055	1.836585130	0.095759005
N	-1.428332105	-1.462862106	-0.335484025
H	-0.981683070	-2.341069169	-0.518969039
H	-2.367879172	-1.333404094	-0.661365048
H	-1.091761077	2.826306201	0.433289030
N	2.650007192	0.602838045	0.026660003
H	3.167996226	1.454907106	0.138451009
H	3.148530229	-0.263370019	0.024171002
O	4.157771300	3.293515239	0.374946026
H	3.473340251	3.954333287	0.314219021
H	4.902083353	3.622495262	-0.110765006
O	-0.129367010	-4.223249306	-0.785449054
H	0.738668055	-4.103348293	-0.412445029
H	-0.025713003	-4.629513333	-1.634728119
O	-4.040894292	-0.778061057	-1.917460135
H	-4.166135301	0.166701010	-1.894304138
H	-4.826296349	-1.160227082	-2.284701166
O	1.657414122	4.625670331	-0.059862007
H	1.277970094	3.752638268	-0.137450012
H	0.953166068	5.252338376	0.012852001
O	2.080660151	-3.069893220	0.584079045
H	2.059085150	-3.233987233	1.519082109
H	1.603828115	-2.248697163	0.442274031
O	-3.749365269	2.008116146	-1.381407101
H	-4.242122307	2.475856176	-0.721087051
H	-2.963764214	1.672113121	-0.959689067
O	4.620017332	-1.883432133	0.126561010
H	5.377901390	-2.234203163	-0.320298024
H	3.955745285	-2.563455183	0.170168015

Coord_6

C	-0.693250052	-0.367202025	-0.124961011
N	0.638493045	-0.524310035	0.079762008
C	1.318107093	0.647727045	0.078754005
C	-0.615094044	1.877631134	0.443494033
N	-1.317036097	0.810141057	-0.125130009
N	0.739893052	1.847747134	0.095217006
N	-1.430157105	-1.459982107	-0.333083026
H	-0.978779072	-2.336037170	-0.514943037
H	-2.369353169	-1.336056098	-0.662512045
H	-1.093099080	2.842149207	0.369772027
N	2.649393193	0.605410042	0.036685001
H	3.171665229	1.455221104	0.146151009

H	3.143572225	-0.263169017	0.035488002
O	4.170863299	3.289749237	0.367964025
H	3.486013253	3.950687282	0.311852022
H	4.912034351	3.618883262	-0.122406011
O	-0.129065008	-4.219921305	-0.787799056
H	0.739967053	-4.106137296	-0.415516030
H	-0.029578002	-4.630210334	-1.635659116
O	-4.042636290	-0.788980058	-1.918615139
H	-4.173181301	0.155039012	-1.892191139
H	-4.828991349	-1.174730084	-2.279980164
O	1.673586123	4.628572334	-0.053991002
H	1.294183096	3.754115270	-0.120671008
H	0.971993073	5.249693379	0.071296003
O	2.080811151	-3.069964220	0.585871040
H	2.060830149	-3.234187235	1.520924111
H	1.603890113	-2.249371161	0.444924034
O	-3.766878269	1.995438144	-1.377429101
H	-4.261449305	2.465347176	-0.720024050
H	-2.982198215	1.661030117	-0.952484070
O	4.622079335	-1.885428137	0.128494010
H	5.378573387	-2.230178161	-0.325406024
H	3.959586287	-2.567183184	0.168383010

Coord_7

C	-0.700782049	-0.358527027	-0.127791009
N	0.633975046	-0.513913036	0.078744004
C	1.317401097	0.658884049	0.078936005
C	-0.618592043	1.892650136	0.407176027
N	-1.326198097	0.814702057	-0.132733011
N	0.744547055	1.858680132	0.092620005
N	-1.431655100	-1.457285107	-0.329869025
H	-0.975627070	-2.331264166	-0.509774039
H	-2.370615172	-1.339128099	-0.662473045
H	-1.092704081	2.856479205	0.304666022
N	2.649191190	0.607778041	0.044528001
H	3.175912231	1.455279102	0.150997013
H	3.138935224	-0.263193020	0.044892006
O	4.180965303	3.289081236	0.367941026
H	3.495444250	3.949506286	0.312300023
H	4.920348355	3.617460262	-0.125612010
O	-0.129531007	-4.216628304	-0.788683057
H	0.740707054	-4.108964298	-0.417722032
H	-0.034827002	-4.631146332	-1.635064120
O	-4.046321290	-0.797871056	-1.920199136
H	-4.181297303	0.145474011	-1.889989137
H	-4.834185350	-1.186414085	-2.275181162
O	1.687232122	4.631672334	-0.053118003

H	1.309739092	3.755233268	-0.107370006
H	0.990798069	5.245064380	0.126744010
O	2.081250151	-3.070096223	0.587406040
H	2.063419148	-3.234263235	1.522547109
H	1.604284118	-2.250064160	0.447462032
O	-3.783367273	1.984208141	-1.372867101
H	-4.278898311	2.456247174	-0.717759050
H	-2.999575216	1.650421119	-0.945493067
O	4.624386331	-1.887974136	0.128679010
H	5.379154386	-2.226919159	-0.332484024
H	3.963542284	-2.571271184	0.165270014

Coord_8

C	-0.707928053	-0.349990027	-0.130896009
N	0.629998046	-0.503635038	0.076810004
C	1.317345094	0.669880050	0.076924004
C	-0.620603044	1.906827139	0.369042027
N	-1.334554097	0.819327061	-0.141031013
N	0.749615055	1.869308133	0.087333005
N	-1.432875103	-1.454799107	-0.325592024
H	-0.972339070	-2.326822167	-0.503153037
H	-2.371766170	-1.342669099	-0.660867045
H	-1.090411077	2.869259206	0.237492019
N	2.649513189	0.609737045	0.049497001
H	3.180923227	1.454845103	0.152081012
H	3.134665224	-0.263680017	0.051765002
O	4.187643303	3.291998236	0.377656028
H	3.501231253	3.951179285	0.316823023
H	4.927199354	3.618203259	-0.117070010
O	-0.130925008	-4.213470301	-0.787654056
H	0.740817054	-4.111883298	-0.418856032
H	-0.041835002	-4.632421331	-1.632504119
O	-4.052245292	-0.804883057	-1.921665137
H	-4.190653300	0.137889012	-1.887382135
H	-4.842202349	-1.195415089	-2.269696165
O	1.698334123	4.634883334	-0.058866005
H	1.324999098	3.755874271	-0.098593008
H	1.010115070	5.238114377	0.178168011
O	2.082148149	-3.070265221	0.588509041
H	2.067255149	-3.234207233	1.523770111
H	1.605115116	-2.250777163	0.449835032
O	-3.798797272	1.974411143	-1.367826101
H	-4.294430308	2.448733175	-0.714527052
H	-3.015901218	1.640289121	-0.938696065
O	4.626894334	-1.890796137	0.126430007
H	5.379532388	-2.224035159	-0.342398027
H	3.967644286	-2.575529188	0.160258012

Coord_9

C	-0.714696050	-0.341613024	-0.134331010
N	0.626582043	-0.493564033	0.073657007
C	1.318076094	0.680548047	0.071993004
C	-0.620886042	1.920179138	0.328528021
N	-1.342026095	0.824047057	-0.150194013
N	0.755367052	1.879522138	0.078470006
N	-1.433941104	-1.452511103	-0.319906025
H	-0.969141072	-2.322771167	-0.494653037
H	-2.372996168	-1.346669097	-0.657162048
H	-1.085972079	2.880453205	0.167563013
N	2.650489193	0.610976045	0.050621006
H	3.186939232	1.453552106	0.148126010
H	3.130792224	-0.264993016	0.055244004
O	4.190106300	3.299589236	0.400873028
H	3.502661254	3.956508285	0.327097026
H	4.932598354	3.621626263	-0.092183005
O	-0.133540011	-4.210563303	-0.784077056
H	0.740134056	-4.114955299	-0.418622030
H	-0.051196004	-4.634156334	-1.627354118
O	-4.060896292	-0.810049060	-1.922349141
H	-4.201516303	0.132303012	-1.883995136
H	-4.853581347	-1.201687088	-2.262796165
O	1.706841124	4.638023334	-0.073526004
H	1.340484094	3.755847273	-0.095797005
H	1.030845076	5.228379379	0.224121017
O	2.083689151	-3.070441220	0.588930044
H	2.072842149	-3.234009230	1.524338109
H	1.606484114	-2.251511164	0.451972035
O	-3.813069272	1.966154142	-1.362455100
H	-4.307936309	2.443158176	-0.710656052
H	-3.031170220	1.630718119	-0.932067067
O	4.629498331	-1.893557136	0.120779008
H	5.379489387	-2.221049160	-0.356360025
H	3.971880286	-2.579717186	0.152541010

Coord_10

C	-0.731234051	-0.314892023	-0.147504009
N	0.612614044	-0.457730033	0.071083004
C	1.304521092	0.719073050	0.055041006
C	-0.640272049	1.956903140	0.246679017
N	-1.362549097	0.844774062	-0.189412011
N	0.742697052	1.915476139	0.037107004
N	-1.439955103	-1.436603104	-0.312212021
H	-0.967002069	-2.305846168	-0.468877036
H	-2.377382169	-1.345109098	-0.658476048

H	-1.102198082	2.909950211	0.040022003
N	2.637389188	0.644079045	0.049031003
H	3.175752229	1.486971110	0.132770011
H	3.115468224	-0.232716014	0.071452005
O	4.159411300	3.357752239	0.421177030
H	3.469404252	4.006867290	0.310315021
H	4.911038355	3.669411265	-0.064659004
O	-0.129604007	-4.195390304	-0.731691054
H	0.743669055	-4.097722292	-0.366190027
H	-0.047989005	-4.634456335	-1.567161111
O	-4.068419293	-0.830050060	-1.948275143
H	-4.213296302	0.112064009	-1.919583136
H	-4.860729352	-1.228902086	-2.281075164
O	1.684555120	4.668113337	-0.157044012
H	1.332056094	3.780991272	-0.148714010
H	1.021807072	5.244844380	0.193636015
O	2.080368151	-3.032182218	0.634617044
H	2.068977150	-3.183119228	1.572156116
H	1.600853117	-2.217422158	0.486030036
O	-3.835279275	1.950913139	-1.418342102
H	-4.334950310	2.437948178	-0.777909056
H	-3.056635218	1.621561114	-0.976900070
O	4.625461333	-1.854401136	0.159633011
H	5.376740385	-2.179487156	-0.317226023
H	3.971890287	-2.544037183	0.194507014

LIIC path connecting T1-MIN and T₁/S₀
Coord_1

C	-0.731234051	-0.314892023	-0.147504009
N	0.612614044	-0.457730033	0.071083004
C	1.304521092	0.719073050	0.055041006
C	-0.640272049	1.956903140	0.246679017
N	-1.362549097	0.844774062	-0.189412011
N	0.742697052	1.915476139	0.037107004
N	-1.439955103	-1.436603104	-0.312212021
H	-0.967002069	-2.305846168	-0.468877036
H	-2.377382169	-1.345109098	-0.658476048
H	-1.102198082	2.909950211	0.040022003
N	2.637389188	0.644079045	0.049031003
H	3.175752229	1.486971110	0.132770011
H	3.115468224	-0.232716014	0.071452005
O	4.159411300	3.357752239	0.421177030
H	3.469404252	4.006867290	0.310315021
H	4.911038355	3.669411265	-0.064659004
O	-0.129604007	-4.195390304	-0.731691054
H	0.743669055	-4.097722292	-0.366190027
H	-0.047989005	-4.634456335	-1.567161111

O	-4.068419293	-0.830050060	-1.948275143
H	-4.213296302	0.112064009	-1.919583136
H	-4.860729352	-1.228902086	-2.281075164
O	1.684555120	4.668113337	-0.157044012
H	1.332056094	3.780991272	-0.148714010
H	1.021807072	5.244844380	0.193636015
O	2.080368151	-3.032182218	0.634617044
H	2.068977150	-3.183119228	1.572156116
H	1.600853117	-2.217422158	0.486030036
O	-3.835279275	1.950913139	-1.418342102
H	-4.334950310	2.437948178	-0.777909056
H	-3.056635218	1.621561114	-0.976900070
O	4.625461333	-1.854401136	0.159633011
H	5.376740385	-2.179487156	-0.317226023
H	3.971890287	-2.544037183	0.194507014

Coord_2

C	-0.716952049	-0.329212025	-0.165263013
N	0.617977044	-0.464837032	0.065272003
C	1.300698093	0.723232050	0.053610005
C	-0.645609045	1.946529138	0.280494020
N	-1.344853098	0.843651058	-0.238152019
N	0.733772054	1.917484139	0.059227005
N	-1.442006104	-1.442764103	-0.312638025
H	-0.977627069	-2.321634166	-0.444483034
H	-2.376244174	-1.354609100	-0.671879049
H	-1.119216078	2.902367207	0.117544010
N	2.632170188	0.653161050	0.033549001
H	3.169073229	1.496848108	0.119233011
H	3.112239222	-0.222809017	0.048142006
O	4.164156300	3.367462245	0.409046028
H	3.468440250	4.009046288	0.292739023
H	4.916965352	3.688731267	-0.068964004
O	-0.139601012	-4.194157300	-0.717344053
H	0.735568055	-4.092131297	-0.356944025
H	-0.059547003	-4.621856334	-1.558837111
O	-4.076510291	-0.832376058	-1.933974138
H	-4.223179307	0.110188007	-1.912136136
H	-4.869768350	-1.233724087	-2.260269164
O	1.675912121	4.665762334	-0.156434013
H	1.322547097	3.778341274	-0.135763011
H	1.034992074	5.240510376	0.235891019
O	2.080220150	-3.033943220	0.635828045
H	2.068760150	-3.183957228	1.573450113
H	1.603902115	-2.216970161	0.486656037
O	-3.849035275	1.960848140	-1.457398103
H	-4.321189310	2.477109178	-0.818948059

H	-3.046042217	1.664373120	-1.040602072
O	4.618599333	-1.844177135	0.157788014
H	5.373826386	-2.173626158	-0.309730021
H	3.967009284	-2.535403185	0.198326012

Coord_3

C	-0.701978053	-0.344753024	-0.181322013
N	0.623730047	-0.473184036	0.060294006
C	1.296869094	0.726191050	0.052958006
C	-0.651659049	1.929928139	0.317573020
N	-1.324032095	0.841145060	-0.284744023
N	0.723882054	1.917092140	0.083129004
N	-1.443561102	-1.449094105	-0.311609024
H	-0.988872070	-2.337051169	-0.419057030
H	-2.374111171	-1.361879095	-0.683389051
H	-1.139061082	2.885439208	0.199173014
N	2.626760192	0.661652048	0.017254999
H	3.162025228	1.506273109	0.104475009
H	3.109095226	-0.213276016	0.023172000
O	4.164481299	3.375942242	0.393594026
H	3.462925249	4.010080290	0.273174017
H	4.917523353	3.706506267	-0.077885006
O	-0.148456010	-4.195069300	-0.702198053
H	0.728488055	-4.088046292	-0.347005023
H	-0.069933007	-4.611443332	-1.549494111
O	-4.080012296	-0.830584058	-1.920675136
H	-4.226764302	0.112584010	-1.904695137
H	-4.874383353	-1.232847087	-2.242120162
O	1.662265121	4.661844338	-0.155867010
H	1.309599093	3.773781269	-0.122408011
H	1.045199078	5.233252376	0.277647020
O	2.080603148	-3.036287221	0.637184045
H	2.069382150	-3.185211230	1.574922115
H	1.607423118	-2.217162158	0.487448035
O	-3.855011279	1.973119141	-1.493796110
H	-4.300560308	2.516929184	-0.859084063
H	-3.029198220	1.707954121	-1.104538077
O	4.611505331	-1.833423132	0.155397011
H	5.370791385	-2.166644156	-0.302759021
H	3.962256288	-2.526542181	0.201741016

Coord_4

C	-0.686385052	-0.361688025	-0.195594013
N	0.629846045	-0.482907033	0.056230004
C	1.292922093	0.727878051	0.053072001
C	-0.658337049	1.906563138	0.357714025
N	-1.299900094	0.837194059	-0.329093024

N	0.712909050	1.914138135	0.108715010
N	-1.444649106	-1.455762103	-0.309193022
H	-1.000755073	-2.352287171	-0.392713031
H	-2.370918169	-1.367126100	-0.693320052
H	-1.161733084	2.858365204	0.284633023
N	2.620990191	0.669642047	0.000092998
H	3.154355227	1.515401110	0.088346004
H	3.105939224	-0.203961015	-0.003461999
O	4.160108300	3.383260244	0.374964029
H	3.452532250	4.009965289	0.251568017
H	4.912528354	3.722787268	-0.091227009
O	-0.156058011	-4.198246300	-0.686088051
H	0.722533054	-4.085566292	-0.336233022
H	-0.079070003	-4.603392329	-1.538952111
O	-4.078833295	-0.824342058	-1.908710137
H	-4.223807302	0.119587010	-1.897299138
H	-4.874573349	-1.225728087	-2.227136159
O	1.643352120	4.656191333	-0.155626012
H	1.292997093	3.767142270	-0.108881008
H	1.052207078	5.223043378	0.318299025
O	2.081632149	-3.039241221	0.638745044
H	2.071005148	-3.186834227	1.576643115
H	1.611517119	-2.218037157	0.488422033
O	-3.852723275	1.988124142	-1.527147109
H	-4.272440306	2.557351182	-0.897117064
H	-3.005553215	1.752443127	-1.168624083
O	4.604277330	-1.822239129	0.152342012
H	5.367713389	-2.158694157	-0.296437020
H	3.957721286	-2.517530181	0.204712012

Coord_5

C	-0.670253046	-0.380236026	-0.207983016
N	0.636287048	-0.494175037	0.053171005
C	1.288722092	0.728195055	0.053936005
C	-0.665526049	1.875832137	0.400626030
N	-1.272245090	0.831691060	-0.371096029
N	0.700709049	1.908430138	0.135841012
N	-1.445325103	-1.462960105	-0.305503022
H	-1.013347073	-2.367564169	-0.365634025
H	-2.366578169	-1.370523100	-0.702028050
H	-1.187194087	2.820233204	0.373520026
N	2.614658188	0.677202048	-0.017976003
H	3.145756224	1.524382110	0.070692006
H	3.102645222	-0.194719013	-0.031723001
O	4.150701301	3.389469245	0.353340026
H	3.436885246	4.008665291	0.227864014
H	4.901738350	3.737596267	-0.108740008

O	-0.162270013	-4.203835301	-0.668825051
H	0.717829049	-4.084810293	-0.324464025
H	-0.086853005	-4.597913328	-1.527001109
O	-4.072797293	-0.813305061	-1.898444135
H	-4.213972305	0.131528011	-1.889955137
H	-4.870242350	-1.211793087	-2.215867160
O	1.618866115	4.648570334	-0.156093011
H	1.272487093	3.758203270	-0.095503005
H	1.055707077	5.209834373	0.357093025
O	2.083440152	-3.042837218	0.640577045
H	2.073817148	-3.188773228	1.578694111
H	1.616300119	-2.219641157	0.489594034
O	-3.841571277	2.006242145	-1.556920113
H	-4.236046304	2.598240189	-0.931571069
H	-2.974442212	1.798013130	-1.232757090
O	4.597021331	-1.810730133	0.148486009
H	5.364679388	-2.149935157	-0.290906022
H	3.953505283	-2.508444181	0.207192017

Coord_6

C	-0.653678045	-0.400663030	-0.218390017
N	0.643002048	-0.507202037	0.051216002
C	1.284104095	0.727003051	0.055521002
C	-0.673071047	1.837066131	0.445916030
N	-1.240841087	0.824462059	-0.410656029
N	0.687101049	1.899735137	0.164308012
N	-1.445663105	-1.470923106	-0.300693023
H	-1.026765072	-2.383152170	-0.338070024
H	-2.360971171	-1.372233099	-0.709902054
H	-1.215358086	2.770017199	0.465272032
N	2.607519185	0.684376051	-0.036990003
H	3.135863223	1.533345108	0.051349005
H	3.099059221	-0.185427015	-0.061540007
O	4.135872300	3.394588247	0.328954025
H	3.415556244	4.006090288	0.202000016
H	4.884858353	3.750920272	-0.130117007
O	-0.166930011	-4.212019302	-0.650175045
H	0.714531053	-4.085923296	-0.311501024
H	-0.093151008	-4.595267331	-1.513385108
O	-4.061616291	-0.797135055	-1.890273136
H	-4.196792301	0.148706009	-1.882633134
H	-4.861165352	-1.190448088	-2.208895160
O	1.588448113	4.638670333	-0.157767011
H	1.247765091	3.746678271	-0.082689004
H	1.055273078	5.193549371	0.393132028
O	2.086175151	-3.047117220	0.642766045
H	2.078028150	-3.190963228	1.581174116

H	1.621899116	-2.222034160	0.490983034
O	-3.820793276	2.027804144	-1.582403115
H	-4.190366301	2.639327188	-0.960630071
H	-2.935059212	1.844869135	-1.296816091
O	4.589846328	-1.799005131	0.143671009
H	5.361779386	-2.140530153	-0.286328020
H	3.949720285	-2.499366182	0.209126017

Coord_7

C	-0.636776044	-0.423297031	-0.226723018
N	0.649919045	-0.522249038	0.050457003
C	1.278871093	0.724120051	0.057764004
C	-0.680780048	1.789523127	0.493078037
N	-1.205444088	0.815253057	-0.447685032
N	0.671853050	1.887771138	0.193842013
N	-1.445748107	-1.479942106	-0.294966023
H	-1.041162074	-2.399382174	-0.310349021
H	-2.353929171	-1.372417099	-0.717374052
H	-1.246086091	2.706576197	0.559154039
N	2.599285187	0.691170052	-0.057002005
H	3.124245227	1.542391113	0.030118001
H	3.094991224	-0.175998013	-0.092833009
O	4.115168298	3.398592245	0.302089024
H	3.388057241	4.002086290	0.173905012
H	4.861538348	3.762692270	-0.154981009
O	-0.169844010	-4.223034301	-0.629851046
H	0.712816053	-4.089091295	-0.297098020
H	-0.097799010	-4.595792333	-1.497788106
O	-4.044861290	-0.775510057	-1.884634138
H	-4.171650301	0.171375010	-1.875257133
H	-4.846942348	-1.161096081	-2.206820161
O	1.551676110	4.626084333	-0.161280012
H	1.218466087	3.732202268	-0.070968003
H	1.050343077	5.174073373	0.425356033
O	2.089998150	-3.052128221	0.645417048
H	2.083870150	-3.193321231	1.584205117
H	1.628448118	-2.225289161	0.492611038
O	-3.789374271	2.053054148	-1.602663115
H	-4.134070298	2.680125193	-0.982070073
H	-2.886420207	1.893259135	-1.360659098
O	4.582858331	-1.787179131	0.137720009
H	5.359103384	-2.130649155	-0.282872021
H	3.946478286	-2.490382182	0.210461015

Coord_8

C	-0.619683042	-0.448537034	-0.232920017
N	0.656944048	-0.539639041	0.050963002

C	1.272780093	0.719305052	0.060546005
C	-0.688413049	1.732385123	0.541467041
N	-1.165799086	0.803710056	-0.482129036
N	0.654667046	1.872194134	0.224067014
N	-1.445686103	-1.490368105	-0.288599021
H	-1.056737078	-2.416652175	-0.282893019
H	-2.345222168	-1.371241098	-0.724936053
H	-1.279177089	2.628639189	0.654232046
N	2.589605186	0.697536049	-0.078116008
H	3.110386223	1.551578111	0.006731002
H	3.090203223	-0.166391012	-0.125542011
O	4.088068295	3.401398244	0.273069018
H	3.353829242	3.996411287	0.143490009
H	4.831372350	3.772785273	-0.182890013
O	-0.170784014	-4.237187306	-0.607488042
H	0.712891053	-4.094548293	-0.280936021
H	-0.100587006	-4.599930330	-1.479805108
O	-4.021931288	-0.748127056	-1.882013134
H	-4.137765299	0.199732015	-1.867722136
H	-4.826960345	-1.123155083	-2.210222157
O	1.508042106	4.610287334	-0.167418013
H	1.184140084	3.714315267	-0.061008004
H	1.040177074	5.151229373	0.452539032
O	2.095071150	-3.057925220	0.648678045
H	2.091579152	-3.195724230	1.587953115
H	1.636075118	-2.229493162	0.494502037
O	-3.745934269	2.082100148	-1.616493115
H	-4.065339291	2.719802194	-0.993175069
H	-2.827316205	1.943474140	-1.424119103
O	4.576148332	-1.775368128	0.130440012
H	5.356732384	-2.120471155	-0.280711020
H	3.943888286	-2.481577180	0.211154015

Coord_9

C	-0.602567042	-0.476858034	-0.236978018
N	0.663945047	-0.559758042	0.052749002
C	1.265529090	0.712255051	0.063647005
C	-0.695682050	1.664746121	0.590274043
N	-1.121647082	0.789361055	-0.513991037
N	0.635154047	1.852587132	0.254464019
N	-1.445610102	-1.502597110	-0.281979019
H	-1.073767076	-2.435413175	-0.256264021
H	-2.334561167	-1.368845100	-0.733172052
H	-1.314345093	2.534804183	0.749338051
N	2.578054183	0.703364053	-0.100530009
H	3.093663222	1.560907114	-0.019209002
H	3.084402223	-0.156621014	-0.159672012

O	4.053971293	3.402861245	0.242248015
H	3.312228237	3.988732285	0.110627007
H	4.793883343	3.781016271	-0.213337014
O	-0.169479010	-4.254882305	-0.582617044
H	0.714994051	-4.102595295	-0.262596018
H	-0.101248007	-4.608268332	-1.458911105
O	-3.992035287	-0.714689049	-1.882978136
H	-4.094221293	0.233923015	-1.859913136
H	-4.800352345	-1.076111078	-2.219605157
O	1.456932104	4.590610328	-0.177161013
H	1.144233081	3.692441265	-0.053647005
H	1.023821073	5.124752371	0.473260036
O	2.101556154	-3.064556219	0.652750048
H	2.101381149	-3.197996231	1.592639117
H	1.644897117	-2.234750162	0.496687036
O	-3.688550267	2.114843154	-1.622367115
H	-3.981613284	2.756982198	-0.990665071
H	-2.756257199	1.995857142	-1.486998108
O	4.569778329	-1.763685127	0.121628009
H	5.354727384	-2.110176149	-0.279997022
H	3.942040283	-2.473032179	0.211191015

Coord_10

C	-0.583986042	-0.586611041	-0.236456017
N	0.675116047	-0.669769050	0.043966004
C	1.257893088	0.615953047	0.105044007
C	-0.698250052	1.467863106	0.731137053
N	-1.077011076	0.704244048	-0.481340033
N	0.613009043	1.729532123	0.376378027
N	-1.441772102	-1.594841114	-0.308966021
H	-1.085941080	-2.533945180	-0.307946022
H	-2.322106166	-1.425755102	-0.761579054
H	-1.347548097	2.294313163	0.977081070
N	2.563516187	0.633873047	-0.097116006
H	3.071164219	1.493141110	0.011731002
H	3.078175220	-0.216028018	-0.208959014
O	4.007537286	3.315622237	0.340353027
H	3.255239234	3.894499279	0.236820017
H	4.738871341	3.721378270	-0.104818006
O	-0.157063009	-4.336186315	-0.717192052
H	0.730230054	-4.184146304	-0.405034029
H	-0.097712008	-4.642859337	-1.611518113
O	-3.966440286	-0.691632050	-1.862146132
H	-4.054438292	0.254635017	-1.784221131
H	-4.780329346	-1.023570074	-2.216650157
O	1.386562097	4.487513323	0.011574001
H	1.090586081	3.581021260	0.117143010

H	0.993620071	4.984803361	0.714637052
O	2.125568153	-3.178070226	0.526254037
H	2.138005152	-3.346116240	1.460483105
H	1.667466119	-2.342475167	0.407295028
O	-3.631619262	2.120906155	-1.474178107
H	-3.892265278	2.730300198	-0.797359056
H	-2.687682193	2.020712147	-1.417312100
O	4.571457329	-1.828783131	0.015413002
H	5.358238385	-2.157029154	-0.397885029
H	3.951416282	-2.546802181	0.089625004

LIIC path connecting T₁/S₀ and S0-MIN
Coord_1

C	-0.583986042	-0.586611041	-0.236456017
N	0.675116047	-0.669769050	0.043966004
C	1.257893088	0.615953047	0.105044007
C	-0.698250052	1.467863106	0.731137053
N	-1.077011076	0.704244048	-0.481340033
N	0.613009043	1.729532123	0.376378027
N	-1.441772102	-1.594841114	-0.308966021
H	-1.085941080	-2.533945180	-0.307946022
H	-2.322106166	-1.425755102	-0.761579054
H	-1.347548097	2.294313163	0.977081070
N	2.563516187	0.633873047	-0.097116006
H	3.071164219	1.493141110	0.011731002
H	3.078175220	-0.216028018	-0.208959014
O	4.007537286	3.315622237	0.340353027
H	3.255239234	3.894499279	0.236820017
H	4.738871341	3.721378270	-0.104818006
O	-0.157063009	-4.336186315	-0.717192052
H	0.730230054	-4.184146304	-0.405034029
H	-0.097712008	-4.642859337	-1.611518113
O	-3.966440286	-0.691632050	-1.862146132
H	-4.054438292	0.254635017	-1.784221131
H	-4.780329346	-1.023570074	-2.216650157
O	1.386562097	4.487513323	0.011574001
H	1.090586081	3.581021260	0.117143010
H	0.993620071	4.984803361	0.714637052
O	2.125568153	-3.178070226	0.526254037
H	2.138005152	-3.346116240	1.460483105
H	1.667466119	-2.342475167	0.407295028
O	-3.631619262	2.120906155	-1.474178107
H	-3.892265278	2.730300198	-0.797359056
H	-2.687682193	2.020712147	-1.417312100
O	4.571457329	-1.828783131	0.015413002
H	5.358238385	-2.157029154	-0.397885029
H	3.951416282	-2.546802181	0.089625004

Coord_2

C	-0.615045042	-0.599601041	-0.212818013
N	0.651874048	-0.666878049	0.044900002
C	1.235008088	0.608857044	0.108188008
C	-0.729912055	1.525845111	0.663268049
N	-1.170256087	0.660571050	-0.435357033
N	0.595734041	1.735027126	0.353508024
N	-1.452217103	-1.628282115	-0.276817022
H	-1.073487078	-2.557821186	-0.301996021
H	-2.342075167	-1.474226108	-0.715368052
H	-1.364043097	2.372923168	0.877698063
N	2.546925183	0.628404048	-0.060709003
H	3.048699221	1.490664105	0.050071005
H	3.066018219	-0.219367015	-0.165291011
O	4.016363291	3.321250238	0.342961024
H	3.265208235	3.904085283	0.258094016
H	4.742018342	3.731255268	-0.107816007
O	-0.157212009	-4.334629311	-0.733325053
H	0.731554055	-4.184386301	-0.424792031
H	-0.102338006	-4.643913336	-1.627062118
O	-3.973866288	-0.687782048	-1.882309134
H	-4.067158295	0.257262017	-1.799625131
H	-4.785091344	-1.022031073	-2.240374163
O	1.395377100	4.493977323	0.042433004
H	1.100923077	3.585357259	0.123383010
H	0.967487070	4.985837358	0.728692053
O	2.124998155	-3.172953230	0.508996037
H	2.141917153	-3.344953241	1.442509103
H	1.658760121	-2.341433169	0.395177028
O	-3.645665261	2.112237152	-1.436288105
H	-3.937467281	2.694040195	-0.758138052
H	-2.725906195	1.972654143	-1.339238099
O	4.584255332	-1.839472130	0.011272999
H	5.361640387	-2.162989155	-0.423064029
H	3.957328287	-2.552669185	0.071272005

Coord_3

C	-0.644111044	-0.607012041	-0.187086013
N	0.630646045	-0.662810046	0.046932005
C	1.216203087	0.602103044	0.110925008
C	-0.754222056	1.575045111	0.591476043
N	-1.248969091	0.625429045	-0.385328029
N	0.581349040	1.739700126	0.329337022
N	-1.463127108	-1.653371118	-0.242851018
H	-1.065362075	-2.573550186	-0.294796020
H	-2.361735171	-1.511738108	-0.666982048

H	-1.374270098	2.440099177	0.774296056
N	2.533323185	0.622414047	-0.026780004
H	3.030142219	1.487340105	0.083743003
H	3.056117217	-0.223651017	-0.123751010
O	4.022590289	3.327653241	0.355184024
H	3.273020235	3.913739280	0.282977021
H	4.743490339	3.738272269	-0.102819007
O	-0.157394009	-4.335226313	-0.745824055
H	0.732989052	-4.185923302	-0.441855034
H	-0.107570008	-4.648054333	-1.638640120
O	-3.981290285	-0.683932050	-1.902471137
H	-4.079877293	0.259889017	-1.815028131
H	-4.789851346	-1.020493072	-2.264097163
O	1.402753101	4.499234324	0.067307007
H	1.109108078	3.589642261	0.129214009
H	0.939785070	4.990484360	0.730807053
O	2.124801153	-3.167519226	0.492236036
H	2.146559154	-3.343014240	1.425059102
H	1.650571119	-2.340186168	0.383322029
O	-3.659711266	2.103567149	-1.398398099
H	-3.982668289	2.657778191	-0.718917054
H	-2.764130197	1.924595138	-1.261163092
O	4.596172330	-1.849465135	0.003896999
H	5.363830387	-2.167279158	-0.451485033
H	3.962737283	-2.557732184	0.050890002

Coord_4

C	-0.671525051	-0.609516045	-0.159707011
N	0.6111110043	-0.657718049	0.049935001
C	1.200956088	0.595613045	0.113608011
C	-0.771859057	1.615673118	0.517374035
N	-1.314780092	0.598873041	-0.332133026
N	0.569644042	1.743584128	0.304445022
N	-1.474279105	-1.671465122	-0.207747013
H	-1.060672077	-2.582395188	-0.286934023
H	-2.380965170	-1.540179109	-0.617283044
H	-1.378592101	2.496394180	0.668947047
N	2.522367184	0.615993042	0.005244999
H	3.015120216	1.483240108	0.113761006
H	3.048205219	-0.228718017	-0.083981006
O	4.026204289	3.333985238	0.374169025
H	3.278635235	3.923187285	0.310457021
H	4.743012344	3.742290270	-0.092415007
O	-0.157378012	-4.337686310	-0.755736053
H	0.734657055	-4.188570300	-0.456934034
H	-0.112863008	-4.654808334	-1.647329120
O	-3.988714287	-0.680081048	-1.922633139

H	-4.092595295	0.262515017	-1.830431132
H	-4.794611343	-1.018954071	-2.287821164
O	1.408558101	4.503793323	0.088028006
H	1.115249080	3.593888257	0.134740011
H	0.911017063	4.997506362	0.724031054
O	2.124792152	-3.161818230	0.475948034
H	2.151503157	-3.340477243	1.408091102
H	1.642706117	-2.338772169	0.371717029
O	-3.673756265	2.094897151	-1.360508098
H	-4.027869292	2.621517188	-0.679696050
H	-2.802353199	1.876536134	-1.183088084
O	4.607322333	-1.858818136	-0.005630001
H	5.365022385	-2.170006157	-0.481821034
H	3.967651287	-2.562041184	0.029226004

Coord_5

C	-0.697117052	-0.607592046	-0.131102007
N	0.593441042	-0.651708045	0.053742003
C	1.189347087	0.589292044	0.116445009
C	-0.782875056	1.648008118	0.442384031
N	-1.368629101	0.580865044	-0.276505019
N	0.560989041	1.746674126	0.279294021
N	-1.485005105	-1.683582122	-0.172165013
H	-1.058187077	-2.585244189	-0.279039021
H	-2.399172175	-1.561004113	-0.567063043
H	-1.376731101	2.542443184	0.563498040
N	2.514279181	0.609057042	0.035713003
H	3.003897218	1.478221106	0.140816008
H	3.042499217	-0.234639018	-0.045847001
O	4.027686292	3.339382243	0.397520029
H	3.282625236	3.931988286	0.339363026
H	4.740848342	3.742657270	-0.079038004
O	-0.156514009	-4.341852311	-0.763835053
H	0.737113052	-4.192225300	-0.470506034
H	-0.117282009	-4.663925338	-1.653908122
O	-3.996138290	-0.676231050	-1.942795142
H	-4.105314298	0.265142017	-1.845835132
H	-4.799372345	-1.017415076	-2.311544169
O	1.413385102	4.507867327	0.105518007
H	1.119919080	3.598100260	0.140004012
H	0.882467061	5.006154362	0.710096050
O	2.125227152	-3.155871225	0.460185035
H	2.156781155	-3.337418238	1.391659101
H	1.635419118	-2.337210171	0.360358028
O	-3.687801264	2.086226148	-1.322618097
H	-4.073070295	2.585255185	-0.640474046
H	-2.840577207	1.828477134	-1.105013077

O	4.618188331	-1.867570135	-0.016374004
H	5.365810388	-2.171270155	-0.512909039
H	3.972491285	-2.565635187	0.006964999

Coord_6

C	-0.720250051	-0.601567046	-0.101665009
N	0.578269044	-0.644839044	0.058161004
C	1.182000085	0.583028040	0.119562006
C	-0.786761059	1.672386118	0.367788025
N	-1.410802104	0.571303039	-0.219029014
N	0.556273040	1.748940127	0.254277018
N	-1.494195109	-1.690508121	-0.136757012
H	-1.056294078	-2.582709186	-0.271782022
H	-2.415312176	-1.575384113	-0.517079035
H	-1.367830101	2.578949186	0.459624033
N	2.509799182	0.601365043	0.064816005
H	2.997326218	1.471944106	0.165397011
H	3.039658217	-0.241694020	-0.009355002
O	4.028028289	3.342833240	0.423089032
H	3.286172237	3.939516282	0.368411026
H	4.737789343	3.738250272	-0.065050002
O	-0.153772013	-4.347647315	-0.770712055
H	0.741301056	-4.196834302	-0.482909033
H	-0.119540008	-4.675278338	-1.658966119
O	-4.003562287	-0.672380048	-1.962957139
H	-4.118033295	0.267769017	-1.861238133
H	-4.804132348	-1.015876075	-2.335267169
O	1.418487101	4.511516326	0.120164009
H	1.124145079	3.602279257	0.145002012
H	0.856117061	5.016005361	0.690044048
O	2.126781155	-3.149680227	0.445037035
H	2.162854157	-3.333860241	1.375861101
H	1.629377115	-2.335506167	0.349243025
O	-3.701847269	2.077556150	-1.284728090
H	-4.118271298	2.548994182	-0.601253042
H	-2.878800209	1.780417129	-1.026938076
O	4.629614332	-1.875740135	-0.027512005
H	5.367165389	-2.171153154	-0.543723040
H	3.978067289	-2.568537184	-0.015266002

Coord_7

C	-0.739893052	-0.591641040	-0.071764007
N	0.566621043	-0.637132048	0.062995006
C	1.180011083	0.576696043	0.123029011
C	-0.782519058	1.689177124	0.294748023
N	-1.441001106	0.570042041	-0.160159013
N	0.556839042	1.750336128	0.229739016

N	-1.500309107	-1.692874120	-0.102185005
H	-1.052951074	-2.575185185	-0.265887019
H	-2.427899176	-1.584349116	-0.468081032
H	-1.350522100	2.606666189	0.358865028
N	2.510131182	0.592522041	0.092670007
H	2.996797215	1.463874105	0.187878011
H	3.040726219	-0.250378019	0.025410001
O	4.028683288	3.343124240	0.448851032
H	3.290999239	3.944957282	0.396223026
H	4.735072341	3.727516271	-0.052795003
O	-0.147788008	-4.355033312	-0.776844055
H	0.748516054	-4.202367305	-0.494396037
H	-0.118042008	-4.688809337	-1.662972118
O	-4.010986289	-0.668530050	-1.983119141
H	-4.130752298	0.270396022	-1.876641133
H	-4.808892345	-1.014337074	-2.358990169
O	1.425694104	4.514698327	0.132010012
H	1.129348082	3.606423260	0.149688009
H	0.834541060	5.026858363	0.664541049
O	2.130495153	-3.143236229	0.430600031
H	2.170572154	-3.329800240	1.360810099
H	1.625618115	-2.333655168	0.338370025
O	-3.715892268	2.068886147	-1.246838089
H	-4.163472301	2.512732178	-0.562032039
H	-2.917024211	1.732358125	-0.948863068
O	4.642771335	-1.883316138	-0.038310004
H	5.370392386	-2.169701155	-0.573348039
H	3.985540288	-2.570744187	-0.036902001

Coord_8

C	-0.754708052	-0.577920041	-0.041751005
N	0.559831042	-0.628567045	0.068044003
C	1.184856087	0.570146040	0.126885009
C	-0.768773054	1.698762122	0.224324014
N	-1.458446106	0.576892040	-0.100243009
N	0.564383041	1.750784124	0.205993013
N	-1.501385109	-1.691248122	-0.069147004
H	-1.045634077	-2.562912184	-0.262143021
H	-2.435028178	-1.588944116	-0.420853031
H	-1.323013096	2.626379189	0.262654021
N	2.516839181	0.581958044	0.119348007
H	3.004143217	1.453253105	0.208582013
H	3.047020221	-0.261418017	0.058332002
O	4.031446292	3.338839238	0.472799033
H	3.299248239	3.947319286	0.421287030
H	4.734220339	3.708509267	-0.044673006
O	-0.136935012	-4.364003316	-0.782635059

H	0.760323057	-4.208809303	-0.505168038
H	-0.110951006	-4.704500337	-1.666323123
O	-4.018411291	-0.664680048	-2.003281144
H	-4.143470301	0.273022022	-1.892044138
H	-4.813652347	-1.012798073	-2.382713170
O	1.437263104	4.517292323	0.140846012
H	1.137219080	3.610526262	0.153971010
H	0.820757057	5.038667361	0.634032043
O	2.137695155	-3.136518223	0.416978030
H	2.181078159	-3.325218237	1.346628096
H	1.625457118	-2.331641167	0.327740024
O	-3.729937267	2.060216150	-1.208948088
H	-4.208673304	2.476471181	-0.522810040
H	-2.955247212	1.684300120	-0.870788061
O	4.659080334	-1.890241136	-0.048081003
H	5.377055389	-2.166905157	-0.600943045
H	3.996344288	-2.572221184	-0.057418002

Coord_9

C	-0.763178053	-0.560430039	-0.011983002
N	0.559420041	-0.619080045	0.073104006
C	1.198285087	0.563188042	0.131148008
C	-0.743857056	1.701500122	0.157488012
N	-1.462008104	0.591614042	-0.039561005
N	0.580860044	1.750145127	0.183333013
N	-1.495024108	-1.686235120	-0.038421004
H	-1.031219072	-2.546013183	-0.261437019
H	-2.434358176	-1.590444116	-0.376289025
H	-1.283135092	2.638883187	0.172336012
N	2.531749184	0.568850043	0.144920010
H	3.021581216	1.438999102	0.227824014
H	3.059994219	-0.275873022	0.089294004
O	4.038300291	3.328384241	0.492815035
H	3.313321237	3.945447284	0.441861034
H	4.736814339	3.678921263	-0.043278005
O	-0.119395008	-4.374599318	-0.788434058
H	0.778479054	-4.216166306	-0.515379037
H	-0.096236005	-4.722396339	-1.669353123
O	-4.025835288	-0.660829050	-2.023443146
H	-4.156189298	0.275649022	-1.907447139
H	-4.818412349	-1.011259072	-2.406437175
O	1.455710106	4.519090324	0.146191010
H	1.149540083	3.614573262	0.157699011
H	0.818078060	5.051508366	0.598772043
O	2.149886155	-3.129483224	0.404281030
H	2.195689156	-3.320071237	1.333443095
H	1.630388119	-2.329434170	0.317344024

O	-3.743982272	2.051546147	-1.171057086
H	-4.253874307	2.440210177	-0.483589036
H	-2.993471214	1.636240116	-0.792713059
O	4.680103340	-1.896396134	-0.056148003
H	5.388879389	-2.162685154	-0.625681044
H	4.012077288	-2.572880184	-0.076287007

Coord_10

C	-0.724575054	-0.309980020	-0.139502008
N	0.596051045	-0.422714031	0.010687999
C	1.291079095	0.718973051	0.047564002
C	-0.585017043	1.924243140	-0.179204013
N	-1.364910096	0.864947061	-0.241782016
N	0.723508053	1.932063141	-0.030508000
N	-1.479571105	-1.423341101	-0.151859011
H	-1.025196072	-2.298364163	-0.328535022
H	-2.398063173	-1.320673095	-0.540962037
H	-1.068956077	2.887504206	-0.270127020
N	2.619836188	0.670232048	0.167373012
H	3.142204227	1.522697109	0.228523015
H	3.112959226	-0.196570012	0.195986012
O	4.196028301	3.388554245	0.450144034
H	3.509951252	4.037529291	0.319436021
H	4.934617355	3.657894262	-0.078955008
O	-0.154320013	-4.218779304	-0.696605052
H	0.730803052	-4.073099294	-0.379006028
H	-0.091825006	-4.624088335	-1.550617109
O	-4.089339294	-0.773988054	-1.965449140
H	-4.234864308	0.167451012	-1.951386139
H	-4.873874353	-1.176264085	-2.312571165
O	1.704712122	4.665816337	-0.139021012
H	1.354118097	3.778486274	-0.097140009
H	1.048312074	5.256706380	0.199363015
O	2.076288152	-2.969283216	0.563773042
H	2.057823147	-3.110214224	1.502694109
H	1.587190115	-2.162249154	0.401539030
O	-3.845299278	2.013992146	-1.364224097
H	-4.393147319	2.444727176	-0.722446052
H	-3.116447223	1.616960114	-0.894529064
O	4.683892339	-1.866649134	0.208595015
H	5.408847389	-2.179117155	-0.315210022
H	3.988624285	-2.514204180	0.170493014

For 2-AT

S0-MIN

C	2.010404145	2.225413158	0.765495055
N	0.733465052	1.970661140	0.527942038

C	0.473481037	0.886914066	-0.219420018
C	2.683538196	0.459482034	-0.411087028
N	3.035677217	1.507145108	0.318932022
N	1.446775102	0.107636007	-0.709087052
H	3.471976249	-0.166874013	-0.800625058
N	-0.794624056	0.576531040	-0.514996040
H	-0.974985073	-0.343057027	-0.869526064
H	-1.541119113	1.064285077	-0.057112005
H	2.243360162	3.084142222	1.377352101
O	-1.151952084	3.867401276	1.967531141
H	-0.511431036	3.323101237	1.519413109
H	-0.955890071	4.768363342	1.748159125
O	-3.108885222	2.151434157	0.743146053
H	-3.878275281	1.877573136	1.223994089
H	-2.688481193	2.843955204	1.246873089
O	-0.991563074	-2.610662186	-1.235090089
H	-0.096889005	-2.891674207	-1.401037101
H	-1.415368104	-3.306666240	-0.748383056
O	4.834936348	3.676631264	2.879494209
H	5.122060367	3.616109262	3.780013273
H	5.373438388	3.071854219	2.378706171
O	5.880408423	1.667978119	1.026812073
H	4.971025359	1.635707118	0.740742054
H	6.411359463	1.811739131	0.255726017
O	1.965991140	-2.557345186	-1.762375127
H	2.207905159	-2.559217182	-2.678387195
H	1.716794122	-1.666433123	-1.540605113

S1-MIN

C	2.035513145	2.228362162	0.822884058
N	0.743864051	2.020331145	0.603730042
C	0.531622037	0.899398066	-0.138366007
C	2.709915195	0.898875065	-0.956046067
N	3.027953219	1.569674110	0.231588015
N	1.513038111	0.214646013	-0.739703051
H	3.504027251	0.343978023	-1.430275101
N	-0.697489048	0.429476032	-0.223432017
H	-0.869588062	-0.433855032	-0.709117051
H	-1.465534107	0.936715069	0.183437013
H	2.325074168	2.974204215	1.549250112
O	-1.184937083	3.828100277	1.953210139
H	-0.504848034	3.293568236	1.547056112
H	-0.998707073	4.731003338	1.733732123
O	-3.031856219	2.048767146	0.716246053
H	-3.834117276	1.816593131	1.164605082
H	-2.634817190	2.773471197	1.196510089
O	-0.986562068	-2.490214178	-1.246802089

H	-0.086706004	-2.765346199	-1.404729101
H	-1.402884099	-3.178712229	-0.744633052
O	4.804972348	3.635352264	2.879658206
H	5.070462368	3.608760260	3.788691272
H	5.355823385	3.013705217	2.414794175
O	5.897555422	1.539101112	1.150562083
H	5.003932362	1.435003104	0.840745060
H	6.452144466	1.607066113	0.385298030
O	1.923135138	-2.582725188	-1.583203114
H	2.317628168	-2.567490186	-2.444150177
H	1.853648133	-1.680706123	-1.287718095

S2-MIN

C	2.036715145	2.118517152	0.743930056
N	0.686605052	1.995646143	0.532741041
C	0.315451025	0.960504068	-0.204825013
C	2.591971185	0.714465054	-0.949486069
N	2.995698215	1.504382110	0.101718006
N	1.300239095	0.225188018	-0.725457055
H	3.289289234	0.057686004	-1.435800104
N	-0.951704068	0.616501047	-0.403698031
H	-1.142876080	-0.257077017	-0.854064060
H	-1.685431120	1.103268078	0.077084006
H	2.334283169	2.839158202	1.490787107
O	-1.142089082	3.870173276	1.961443142
H	-0.495685034	3.319576239	1.523747108
H	-0.925355068	4.769077345	1.753469127
O	-3.183215231	2.222876161	0.819226057
H	-3.923897282	1.981517142	1.358319098
H	-2.700484192	2.903183209	1.284867094
O	-0.756807055	-2.405244172	-1.334464094
H	0.170740013	-2.536104181	-1.504013109
H	-1.072007075	-3.188468231	-0.902935066
O	4.878645352	3.621721261	2.887091210
H	5.199803373	3.544917253	3.774676272
H	5.333864386	2.963212214	2.371416172
O	5.791491415	1.552241112	1.006956073
H	4.900191354	1.538340113	0.661959050
H	6.361237456	1.770437127	0.282273019
O	2.293415165	-2.555388183	-1.654684118
H	2.835968205	-3.228916233	-2.045995146
H	2.653949192	-2.369708173	-0.797194058

T1-MIN

C	2.407829171	2.029857145	0.980960071
N	1.038863074	1.949059140	0.591667044
C	0.752902055	0.679947049	0.010798999

C	2.847250206	0.791590055	-0.853764064
N	3.316175238	1.550415112	0.206815016
N	1.604170117	0.163116014	-0.792671059
H	3.586759261	0.340098027	-1.490943109
N	-0.422672030	0.127998007	0.374079027
H	-0.664090047	-0.723259054	-0.102092008
H	-1.185118088	0.759254055	0.542419037
H	2.651867191	2.587215189	1.869896134
O	-0.984758071	3.994929289	1.893237137
H	-0.279822018	3.580436259	1.410837103
H	-0.820116059	4.928731354	1.885988133
O	-2.812620201	2.113047153	0.678807048
H	-3.669201266	1.921617140	1.037650073
H	-2.471278179	2.868816206	1.148115083
O	-0.877262063	-2.707545195	-1.085605078
H	0.021603000	-2.880417205	-1.352890099
H	-1.188104087	-3.489250251	-0.648025046
O	4.883151354	3.608940260	2.901336211
H	5.192565372	3.637391263	3.796362273
H	5.470909392	3.027340220	2.427970175
O	6.100546439	1.601362117	1.185884088
H	5.257464378	1.545553111	0.744722054
H	6.772052487	1.598207115	0.517874039
O	1.992320142	-2.547043185	-1.759953126
H	2.236736159	-2.546465185	-2.674907193
H	1.845557134	-1.638177116	-1.509195109

T2-MIN

C	2.122265151	2.040446146	0.949914067
N	0.761684053	1.880329133	0.642829044
C	0.475079035	0.949734068	-0.183679011
C	2.747535199	0.693868052	-0.752786054
N	3.113343223	1.592034114	0.090076006
N	1.493048107	0.045757004	-0.604504043
H	3.419109246	0.297605020	-1.497190110
N	-0.736964051	0.693320052	-0.724373051
H	-0.912166066	-0.271017022	-0.941882067
H	-1.515604107	1.187469085	-0.324520022
H	2.393918170	2.819733201	1.637142119
O	-1.119728078	3.797204274	1.976554142
H	-0.461732032	3.228349230	1.583424114
H	-0.875372065	4.689700339	1.771962126
O	-3.082905223	2.144201156	0.680635049
H	-3.816185274	1.829165133	1.191529086
H	-2.636442188	2.807073201	1.202426089
O	-0.974682071	-2.576953188	-1.210258087
H	-0.110639009	-2.936941209	-1.382209101

H	-1.442812104	-3.216788231	-0.689396049
O	4.835290346	3.646739264	2.901585210
H	5.101254366	3.575046256	3.807900274
H	5.385072387	3.048730221	2.405655173
O	5.942628428	1.690865120	1.018256071
H	5.096168369	1.713361122	0.583482043
H	6.606958477	1.770834126	0.347697023
O	2.007979142	-2.708548197	-1.672935118
H	2.250285161	-2.557300185	-2.575653184
H	1.830267129	-1.863268136	-1.281926091

T3-MIN

C	2.159525156	2.146813154	0.849934059
N	0.820915058	1.955810140	0.619591045
C	0.538385039	0.884773062	-0.154386012
C	2.764842200	0.756749057	-0.858497062
N	3.130231227	1.560059113	0.200426015
N	1.497756107	0.163105012	-0.749034055
H	3.532873253	0.157731011	-1.318029093
N	-0.720952052	0.502748036	-0.299654020
H	-0.924765067	-0.352255027	-0.786288059
H	-1.467642106	1.030762074	0.118257007
H	2.427501176	2.866196207	1.607485116
O	-1.081122079	3.868295279	1.983440140
H	-0.407631029	3.323690238	1.585034115
H	-0.836236063	4.771686342	1.834106130
O	-2.991633218	2.160985156	0.734857053
H	-3.798673275	1.937483139	1.179014086
H	-2.581367187	2.871687209	1.223432087
O	-1.090580080	-2.428570172	-1.307857094
H	-0.205340013	-2.744370195	-1.470716107
H	-1.534146113	-3.096502221	-0.801254060
O	4.813232344	3.661485264	2.914454208
H	5.097343365	3.598644259	3.815803277
H	5.359868384	3.063690220	2.413600171
O	5.936983429	1.662022118	1.108407077
H	5.057975367	1.603291116	0.742709053
H	6.536211469	1.763481129	0.381963028
O	1.816748132	-2.639875188	-1.619365119
H	2.255167165	-2.630178190	-2.459047178
H	1.773095126	-1.741003124	-1.313036094

S₂/S₁

C	2.060445146	2.282308163	0.775020055
N	0.748986053	1.894929139	0.530101039
C	0.484232034	0.790414060	-0.192116012
C	2.733902196	0.476579036	-0.460365035

N	3.059404218	1.543423109	0.279551021
N	1.459598104	0.044074004	-0.720645050
H	3.538865254	-0.102917006	-0.878035064
N	-0.779972054	0.433360029	-0.386366026
H	-0.964289067	-0.450938033	-0.826183060
H	-1.534823111	0.969351071	0.004144003
H	2.262306163	3.121963224	1.411395100
O	-1.224910090	3.930384281	2.028615145
H	-0.507626035	3.414655246	1.683714120
H	-1.007725073	4.841864347	1.881828134
O	-3.031892219	2.117598151	0.691950049
H	-3.844069275	1.865938137	1.111465082
H	-2.666964190	2.844367206	1.190400086
O	-1.072698075	-2.573787184	-1.307675094
H	-0.172309013	-2.824868204	-1.497719107
H	-1.433421103	-3.250974235	-0.750194054
O	4.835406347	3.711157270	2.904373207
H	5.119665369	3.611883258	3.802531274
H	5.365238384	3.115043226	2.384304173
O	5.902844427	1.719795124	1.041696078
H	5.003443360	1.669064118	0.729622050
H	6.456185465	1.827653131	0.280503022
O	1.866502134	-2.603386189	-1.765776128
H	2.184240157	-2.562330184	-2.657024193
H	1.700955122	-1.706777125	-1.486005107

S₂/T₁

C	2.036715145	2.118517152	0.743930056
N	0.686605052	1.995646143	0.532741041
C	0.315451025	0.960504068	-0.204825013
C	2.591971185	0.714465054	-0.949486069
N	2.995698215	1.504382110	0.101718006
N	1.300239095	0.225188018	-0.725457055
H	3.289289234	0.057686004	-1.435800104
N	-0.951704068	0.616501047	-0.403698031
H	-1.142876080	-0.257077017	-0.854064060
H	-1.685431120	1.103268078	0.077084006
H	2.334283169	2.839158202	1.490787107
O	-1.142089082	3.870173276	1.961443142
H	-0.495685034	3.319576239	1.523747108
H	-0.925355068	4.769077345	1.753469127
O	-3.183215231	2.222876161	0.819226057
H	-3.923897282	1.981517142	1.358319098
H	-2.700484192	2.903183209	1.284867094
O	-0.756807055	-2.405244172	-1.334464094
H	0.170740013	-2.536104181	-1.504013109
H	-1.072007075	-3.188468231	-0.902935066

O	4.878645352	3.621721261	2.887091210
H	5.199803373	3.544917253	3.774676272
H	5.333864386	2.963212214	2.371416172
O	5.791491415	1.552241112	1.006956073
H	4.900191354	1.538340113	0.661959050
H	6.361237456	1.770437127	0.282273019
O	2.293415165	-2.555388183	-1.654684118
H	2.835968205	-3.228916233	-2.045995146
H	2.653949192	-2.369708173	-0.797194058

S₁/T₁

C	2.071994148	2.212038161	0.824554057
N	0.755901056	2.005069144	0.587854042
C	0.515846036	0.897609066	-0.152283009
C	2.715764196	0.852221063	-0.909119063
N	3.066554223	1.594478114	0.216479015
N	1.491892109	0.189024013	-0.737427055
H	3.499197254	0.298619024	-1.400590099
N	-0.729020053	0.455747032	-0.257059020
H	-0.909310064	-0.405588029	-0.742114052
H	-1.490730110	0.971894069	0.148796012
H	2.337757170	2.943288214	1.572777116
O	-1.168031087	3.824687274	1.955171142
H	-0.492052036	3.289524237	1.544481109
H	-0.972845069	4.728738343	1.748396127
O	-3.051377218	2.079015150	0.723462051
H	-3.851062278	1.843580133	1.174689084
H	-2.645065189	2.792651200	1.211820086
O	-1.027388072	-2.478182180	-1.274432089
H	-0.129189010	-2.768451200	-1.413017102
H	-1.460186105	-3.150923227	-0.764899053
O	4.856086351	3.632844260	2.909540210
H	5.093801365	3.583179260	3.825151278
H	5.417602389	3.017360218	2.448599177
O	5.925980427	1.578372112	1.130251080
H	5.038135363	1.536939111	0.788667055
H	6.507685471	1.644897117	0.385593030
O	1.888592135	-2.616299188	-1.556716110
H	2.301075164	-2.610856188	-2.409340173
H	1.818382131	-1.711793122	-1.270388090

S₁/S₀

C	2.031688146	2.264279163	0.855384061
N	0.756042055	2.101385150	0.623201045
C	0.572282043	0.942881069	-0.096529005
C	2.625108190	1.140427085	-1.054436078
N	2.976781213	1.482141108	0.294716019

N	1.619009115	0.255062016	-0.594017041
H	3.404056244	0.721336050	-1.673898120
N	-0.632993046	0.446297032	-0.185591013
H	-0.778891056	-0.438519031	-0.643937046
H	-1.420302100	0.952789066	0.187484012
H	2.367134170	3.010282218	1.562671111
O	-1.219495088	3.865492280	1.955738140
H	-0.515543040	3.357187242	1.556284111
H	-1.057741076	4.776184343	1.749504124
O	-2.995314217	2.039110148	0.686934052
H	-3.800974275	1.791770130	1.121160080
H	-2.623802191	2.775198199	1.170816083
O	-0.896030065	-2.405912173	-1.241652088
H	0.013506000	-2.661313191	-1.383723098
H	-1.313764093	-3.116905226	-0.773223054
O	4.812966348	3.568537259	2.825701203
H	5.114213367	3.577260259	3.724006270
H	5.341484385	2.924589212	2.364425169
O	5.850140421	1.400177103	1.161846084
H	4.955701359	1.198042088	0.906002066
H	6.372034460	1.414289101	0.371180025
O	1.992265145	-2.531771182	-1.412996104
H	2.532767184	-2.547615183	-2.190398156
H	2.003736146	-1.641610116	-1.070561077

T₁/S₀

C	1.960190140	2.363459172	0.892644066
N	0.726979053	2.146382155	0.601789041
C	0.609903043	0.947599070	-0.138174011
C	2.663444193	1.245138091	-0.987650073
N	2.942320211	1.536921113	0.428147030
N	1.637797119	0.343685023	-0.700442052
H	3.511239254	0.842117058	-1.525882111
N	-0.577700040	0.403224031	-0.125317010
H	-0.724321054	-0.487630035	-0.571954043
H	-1.361940099	0.894596063	0.272525019
H	2.251025162	3.158563229	1.566614111
O	-1.316945094	3.855160279	1.960353142
H	-0.611701044	3.378714241	1.530852112
H	-1.192297086	4.774508344	1.766735125
O	-3.003507214	1.954026140	0.671291048
H	-3.822762275	1.688469122	1.067894077
H	-2.684354192	2.712490198	1.156845084
O	-0.824876061	-2.459091179	-1.135401081
H	0.090604009	-2.681868192	-1.295942091
H	-1.194415086	-3.165901229	-0.622222045
O	4.875634349	3.535517255	2.750792200

H	5.162452371	3.558971259	3.653501265
H	5.395831386	2.867035207	2.315225168
O	5.853267419	1.324488098	1.119094082
H	4.966794359	1.055052077	0.904882068
H	6.339486456	1.340098096	0.306075020
O	2.046741148	-2.441023174	-1.437621103
H	2.528015183	-2.502535182	-2.250758161
H	1.991091144	-1.513821108	-1.208409089

LIIC path connecting Franck-Condon point and S1-MIN

Coord_1

C	2.010404145	2.225413158	0.765495055
N	0.733465052	1.970661140	0.527942038
C	0.473481037	0.886914066	-0.219420018
C	2.683538196	0.459482034	-0.411087028
N	3.035677217	1.507145108	0.318932022
N	1.446775102	0.107636007	-0.709087052
H	3.471976249	-0.166874013	-0.800625058
N	-0.794624056	0.576531040	-0.514996040
H	-0.974985073	-0.343057027	-0.869526064
H	-1.541119113	1.064285077	-0.057112005
H	2.243360162	3.084142222	1.377352101
O	-1.151952084	3.867401276	1.967531141
H	-0.511431036	3.323101237	1.519413109
H	-0.955890071	4.768363342	1.748159125
O	-3.108885222	2.151434157	0.743146053
H	-3.878275281	1.877573136	1.223994089
H	-2.688481193	2.843955204	1.246873089
O	-0.991563074	-2.610662186	-1.235090089
H	-0.096889005	-2.891674207	-1.401037101
H	-1.415368104	-3.306666240	-0.748383056
O	4.834936348	3.676631264	2.879494209
H	5.122060367	3.616109262	3.780013273
H	5.373438388	3.071854219	2.378706171
O	5.880408423	1.667978119	1.026812073
H	4.971025359	1.635707118	0.740742054
H	6.411359463	1.811739131	0.255726017
O	1.965991140	-2.557345186	-1.762375127
H	2.207905159	-2.559217182	-2.678387195
H	1.716794122	-1.666433123	-1.540605113

Coord_2

C	2.016752145	2.223324162	0.763047055
N	0.737412053	1.978860143	0.529791036
C	0.474488034	0.889649066	-0.211194016
C	2.694346191	0.478283034	-0.471949031
N	3.037822221	1.505339106	0.306494023

N	1.440514104	0.108563009	-0.712179050
H	3.488921251	-0.138605010	-0.863766064
N	-0.794671058	0.569826042	-0.481035037
H	-0.980287069	-0.344701022	-0.846857063
H	-1.539478108	1.067796078	-0.030499004
H	2.260534165	3.073994222	1.382057100
O	-1.155649085	3.863454281	1.965878139
H	-0.510726034	3.320248241	1.522419111
H	-0.960690069	4.764635341	1.746497127
O	-3.100341222	2.140430155	0.740091055
H	-3.873380281	1.871190136	1.217329086
H	-2.682540194	2.836529202	1.241213088
O	-0.990973073	-2.596846188	-1.236480090
H	-0.095720004	-2.877194209	-1.401539099
H	-1.413938103	-3.292023239	-0.748057056
O	4.813122344	3.687933268	2.861457207
H	5.084353366	3.637646263	3.767548271
H	5.357798385	3.074913223	2.377721171
O	5.882646425	1.649652118	1.054878073
H	4.978985359	1.611373114	0.752729056
H	6.427934464	1.778460126	0.291120021
O	1.961265142	-2.559698183	-1.742561128
H	2.220130159	-2.559661183	-2.652456192
H	1.732026124	-1.667553121	-1.512597111

Coord_3

C	2.021966144	2.222380157	0.760920053
N	0.740478053	1.987526145	0.530740036
C	0.476172035	0.892004063	-0.203364013
C	2.703194194	0.501057035	-0.531596039
N	3.038869220	1.504453110	0.295034023
N	1.436551101	0.110003006	-0.713630049
H	3.502696253	-0.107574009	-0.925937067
N	-0.792989057	0.561588038	-0.448313033
H	-0.982831072	-0.348231026	-0.824618061
H	-1.536915112	1.069293079	-0.006293002
H	2.275518163	3.064983222	1.387146097
O	-1.159345081	3.859506280	1.964224143
H	-0.510021038	3.317395240	1.525425108
H	-0.965490072	4.760905345	1.744835124
O	-3.091795221	2.129425152	0.737035051
H	-3.868483280	1.864806137	1.210664088
H	-2.676598195	2.829103205	1.235553088
O	-0.990383072	-2.583029185	-1.237870090
H	-0.094551004	-2.862713204	-1.402040103
H	-1.412508102	-3.277379238	-0.747731051
O	4.793881343	3.698599264	2.843561205

H	5.050664365	3.658957262	3.754409270
H	5.343588383	3.077341220	2.376377172
O	5.883442424	1.630578115	1.082772080
H	4.985250357	1.585786113	0.766336055
H	6.441658465	1.743564125	0.325820026
O	1.956538140	-2.562050186	-1.722747123
H	2.232355159	-2.560104184	-2.626524189
H	1.747257126	-1.668673119	-1.484588108

Coord_4

C	2.026147147	2.222547160	0.759045057
N	0.742727056	1.996714144	0.530727040
C	0.478568033	0.894019064	-0.195930014
C	2.710124193	0.527713037	-0.589924040
N	3.038882221	1.504358107	0.284494018
N	1.434999104	0.111992009	-0.713456050
H	3.513306252	-0.074076004	-0.986924073
N	-0.789590056	0.551913037	-0.416776032
H	-0.982621068	-0.353594026	-0.802761056
H	-1.533443112	1.068885078	0.015513000
H	2.288461166	3.057094222	1.392557099
O	-1.163042083	3.855557279	1.962570141
H	-0.509316036	3.314541239	1.528431110
H	-0.970289069	4.757175344	1.743173127
O	-3.083250220	2.118420154	0.733979052
H	-3.863587279	1.858422132	1.203999084
H	-2.670657191	2.821677202	1.229892087
O	-0.989793071	-2.569212187	-1.239260091
H	-0.093382004	-2.848232205	-1.402542102
H	-1.411078101	-3.262734236	-0.747406052
O	4.776956344	3.708584267	2.825858205
H	5.020926360	3.680097264	3.740668268
H	5.330674384	3.079185223	2.374647170
O	5.882853423	1.610866114	1.110397080
H	4.989753359	1.558839111	0.781619054
H	6.452469466	1.707170124	0.359609025
O	1.951811142	-2.564402183	-1.702933123
H	2.244580159	-2.560547185	-2.600592186
H	1.762488128	-1.669793118	-1.456580106

Coord_5

C	2.029335149	2.223835162	0.757316055
N	0.744178055	2.006494144	0.529614037
C	0.481712034	0.895722062	-0.188922014
C	2.715161193	0.558166039	-0.646793047
N	3.037879219	1.504949108	0.274842021
N	1.435993105	0.114575008	-0.711647053

H	3.520703256	-0.038477002	-1.046421075
N	-0.784465054	0.540861038	-0.386419028
H	-0.979618072	-0.360795027	-0.781256055
H	-1.529072108	1.066636074	0.034829002
H	2.299420168	3.050373221	1.398167103
O	-1.166739085	3.851609278	1.960917140
H	-0.508610034	3.311687238	1.531436112
H	-0.975089072	4.753446343	1.741511124
O	-3.074705219	2.107416151	0.730924054
H	-3.858691278	1.852038132	1.197334086
H	-2.664715192	2.814250205	1.224232087
O	-0.989202070	-2.555395184	-1.240650091
H	-0.092214004	-2.833750206	-1.403043100
H	-1.409647100	-3.248090235	-0.747080052
O	4.762221340	3.717826268	2.808522200
H	4.995327358	3.701096266	3.726481269
H	5.319005385	3.080493222	2.372546172
O	5.880899425	1.590658116	1.137617079
H	4.992349360	1.530448111	0.798738060
H	6.460162465	1.669447120	0.392151028
O	1.947085139	-2.566753185	-1.683119124
H	2.256805164	-2.560990185	-2.574660183
H	1.777720130	-1.670913121	-1.428571103

Coord_6

C	2.031456144	2.226325158	0.755534056
N	0.744764055	2.016959143	0.527119041
C	0.485616034	0.897105067	-0.182432015
C	2.718307194	0.592321044	-0.702012053
N	3.035796218	1.506169110	0.266055017
N	1.439689101	0.117766010	-0.708150054
H	3.524777254	-0.001263998	-1.103973080
N	-0.777602054	0.528407037	-0.357318026
H	-0.973731071	-0.369951027	-0.760093055
H	-1.523842111	1.062525076	0.051402003
H	2.308278166	3.044995219	1.403713102
O	-1.170435086	3.847660277	1.959263143
H	-0.507905038	3.308834237	1.534442108
H	-0.979888069	4.749716342	1.739849126
O	-3.066159218	2.096411148	0.727868050
H	-3.853795277	1.845655133	1.190668088
H	-2.658773193	2.806824202	1.218572086
O	-0.988612069	-2.541578181	-1.242040092
H	-0.091045009	-2.819269202	-1.403545099
H	-1.408217099	-3.233446233	-0.746754052
O	4.749825342	3.726267270	2.791970202
H	4.974526358	3.721951268	3.712194266

H	5.308720381	3.081321221	2.370192169
O	5.877535424	1.570133113	1.164241082
H	4.992757361	1.500621110	0.817989057
H	6.464320464	1.630655115	0.422937032
O	1.942358142	-2.569106188	-1.663304119
H	2.269030164	-2.561434186	-2.548728186
H	1.792951127	-1.672033120	-1.400562101

Coord_7

C	2.032223144	2.230245160	0.753292053
N	0.744231052	2.028238148	0.522676037
C	0.490230036	0.898084066	-0.176664015
C	2.719528197	0.630039047	-0.755327052
N	3.032417221	1.508060109	0.258093016
N	1.446257106	0.121509008	-0.702836050
H	3.525345251	0.036880003	-1.158901086
N	-0.769020053	0.514366038	-0.329673023
H	-0.964815069	-0.381415028	-0.739257055
H	-1.517872108	1.056369078	0.064713006
H	2.314606169	3.041397221	1.408626100
O	-1.174132082	3.843712276	1.957609141
H	-0.507200036	3.305980236	1.537448110
H	-0.984688072	4.745986341	1.738187123
O	-3.057614218	2.085406151	0.724812051
H	-3.848898276	1.839271133	1.184003085
H	-2.652831188	2.799398200	1.212911085
O	-0.988022074	-2.527761183	-1.243430092
H	-0.089876009	-2.804788203	-1.404046103
H	-1.406787104	-3.218802232	-0.746428053
O	4.740486343	3.733909267	2.777073201
H	4.960008359	3.742585270	3.698545266
H	5.300331382	3.081731222	2.367935170
O	5.872579425	1.549505112	1.190001087
H	4.990463362	1.469620107	0.839846062
H	6.464193467	1.591181112	0.451222032
O	1.937631139	-2.571458185	-1.643490119
H	2.281255164	-2.561877182	-2.522796183
H	1.808183128	-1.673153118	-1.372554098

Coord_8

C	2.030964147	2.236088161	0.749766055
N	0.741996056	2.040516145	0.515223035
C	0.495368035	0.898430064	-0.172001011
C	2.718714195	0.671083050	-0.806446056
N	3.027256218	1.510878110	0.250799017
N	1.455864102	0.125606009	-0.695461050
H	3.522099252	0.074984003	-1.210236089

N	-0.758810054	0.498248035	-0.303840024
H	-0.952648067	-0.395983029	-0.718655053
H	-1.511443107	1.047660075	0.073860004
H	2.317434166	3.040503218	1.411741102
O	-1.177828084	3.839764275	1.955956140
H	-0.506495035	3.303126240	1.540453112
H	-0.989487069	4.742257340	1.736525126
O	-3.049069222	2.074401148	0.721757053
H	-3.844002275	1.832887133	1.177338087
H	-2.646889189	2.791971202	1.207251085
O	-0.987432073	-2.513944180	-1.244820087
H	-0.088707009	-2.790307199	-1.404548102
H	-1.405357103	-3.204158231	-0.746102053
O	4.735999343	3.740911271	2.765480197
H	4.954602359	3.762771271	3.686981267
H	5.295044382	3.081780224	2.366590171
O	5.865598424	1.528977110	1.214579089
H	4.984584361	1.438280103	0.864951062
H	6.458568466	1.551576111	0.476034036
O	1.932904142	-2.573809187	-1.623676119
H	2.293480164	-2.562320183	-2.496864180
H	1.823414130	-1.674272122	-1.344545096

Coord_9

C	2.026453144	2.244778161	0.743432052
N	0.736984054	2.054028147	0.502957035
C	0.500648033	0.897690062	-0.169060013
C	2.715594198	0.715112052	-0.855204061
N	3.019433217	1.515277108	0.243695019
N	1.468659105	0.129697010	-0.685659047
H	3.514501251	0.111744010	-1.256813091
N	-0.747160053	0.479075033	-0.280264019
H	-0.936882067	-0.415145029	-0.697931048
H	-1.505057107	1.035319074	0.077554006
H	2.315014164	3.043999217	1.410909103
O	-1.181525085	3.835816274	1.954302138
H	-0.505789038	3.300273239	1.543459109
H	-0.994287072	4.738527339	1.734863123
O	-3.040524221	2.063396150	0.718701054
H	-3.839106275	1.826503134	1.170673083
H	-2.640948190	2.784545200	1.201591084
O	-0.986842072	-2.500127182	-1.246210088
H	-0.087538009	-2.775826200	-1.405049100
H	-1.403926101	-3.189514229	-0.745776054
O	4.739851340	3.747753268	2.759883201
H	4.962855359	3.781966271	3.679981263
H	5.295104380	3.081456224	2.367733172

O	5.855711419	1.508603108	1.237746088
H	4.973741356	1.408493102	0.893941064
H	6.445742464	1.512459106	0.496465035
O	1.928178139	-2.576161184	-1.603862115
H	2.305705164	-2.562763183	-2.470932177
H	1.838645132	-1.675392120	-1.316537093

Coord_10

C	2.035513145	2.228362162	0.822884058
N	0.743864051	2.020331145	0.603730042
C	0.531622037	0.899398066	-0.138366007
C	2.709915195	0.898875065	-0.956046067
N	3.027953219	1.569674110	0.231588015
N	1.513038111	0.214646013	-0.739703051
H	3.504027251	0.343978023	-1.430275101
N	-0.697489048	0.429476032	-0.223432017
H	-0.869588062	-0.433855032	-0.709117051
H	-1.465534107	0.936715069	0.183437013
H	2.325074168	2.974204215	1.549250112
O	-1.184937083	3.828100277	1.953210139
H	-0.504848034	3.293568236	1.547056112
H	-0.998707073	4.731003338	1.733732123
O	-3.031856219	2.048767146	0.716246053
H	-3.834117276	1.816593131	1.164605082
H	-2.634817190	2.773471197	1.196510089
O	-0.986562068	-2.490214178	-1.246802089
H	-0.086706004	-2.765346199	-1.404729101
H	-1.402884099	-3.178712229	-0.744633052
O	4.804972348	3.635352264	2.879658206
H	5.070462368	3.608760260	3.788691272
H	5.355823385	3.013705217	2.414794175
O	5.897555422	1.539101112	1.150562083
H	5.003932362	1.435003104	0.840745060
H	6.452144466	1.607066113	0.385298030
O	1.923135138	-2.582725188	-1.583203114
H	2.317628168	-2.567490186	-2.444150177
H	1.853648133	-1.680706123	-1.287718095

LIIC path connecting S1-MIN and S₁/S₀

Coord_1

C	2.035513145	2.228362162	0.822884058
N	0.743864051	2.020331145	0.603730042
C	0.531622037	0.899398066	-0.138366007
C	2.709915195	0.898875065	-0.956046067
N	3.027953219	1.569674110	0.231588015
N	1.513038111	0.214646013	-0.739703051
H	3.504027251	0.343978023	-1.430275101

N	-0.697489048	0.429476032	-0.223432017
H	-0.869588062	-0.433855032	-0.709117051
H	-1.465534107	0.936715069	0.183437013
H	2.325074168	2.974204215	1.549250112
O	-1.184937083	3.828100277	1.953210139
H	-0.504848034	3.293568236	1.547056112
H	-0.998707073	4.731003338	1.733732123
O	-3.031856219	2.048767146	0.716246053
H	-3.834117276	1.816593131	1.164605082
H	-2.634817190	2.773471197	1.196510089
O	-0.986562068	-2.490214178	-1.246802089
H	-0.086706004	-2.765346199	-1.404729101
H	-1.402884099	-3.178712229	-0.744633052
O	4.804972348	3.635352264	2.879658206
H	5.070462368	3.608760260	3.788691272
H	5.355823385	3.013705217	2.414794175
O	5.897555422	1.539101112	1.150562083
H	5.003932362	1.435003104	0.840745060
H	6.452144466	1.607066113	0.385298030
O	1.923135138	-2.582725188	-1.583203114
H	2.317628168	-2.567490186	-2.444150177
H	1.853648133	-1.680706123	-1.287718095

Coord_2

C	2.033514146	2.228713160	0.824324060
N	0.744010051	2.024792146	0.604183044
C	0.534017041	0.900373065	-0.135852008
C	2.702719194	0.919611066	-0.972993069
N	3.022953219	1.558868110	0.236478015
N	1.520749107	0.213621013	-0.728006054
H	3.496536249	0.378456027	-1.463626106
N	-0.692782048	0.428067029	-0.220390016
H	-0.862899060	-0.437321032	-0.703497051
H	-1.462320107	0.935385067	0.183941012
H	2.327811168	2.974613216	1.548831110
O	-1.186982083	3.827912276	1.955205142
H	-0.504940037	3.296145239	1.548659111
H	-1.003175075	4.731767343	1.737618126
O	-3.028457218	2.045101149	0.715499050
H	-3.830754275	1.811398129	1.163031081
H	-2.633303188	2.770566199	1.196227085
O	-0.985957071	-2.481038176	-1.250668089
H	-0.085830004	-2.755976201	-1.408130103
H	-1.403479100	-3.171434227	-0.752103055
O	4.798910347	3.633177260	2.869689205
H	5.065248363	3.611546262	3.778620273
H	5.349465383	3.009159219	2.407561174

O	5.893078424	1.528245109	1.153200085
H	5.000204361	1.411953101	0.845680061
H	6.446629466	1.589923115	0.386561028
O	1.921424139	-2.583295186	-1.571045113
H	2.332380169	-2.571450183	-2.424293177
H	1.863507133	-1.681766123	-1.270877093

Coord_3

C	2.031226148	2.229422163	0.825833057
N	0.743756052	2.029807148	0.604696044
C	0.536178036	0.901777067	-0.133231009
C	2.694185194	0.941458069	-0.989192069
N	3.017155220	1.547891111	0.241273017
N	1.528656111	0.213443014	-0.715808053
H	3.487335249	0.414365032	-1.496242110
N	-0.688235050	0.426940030	-0.217376018
H	-0.856189061	-0.440558031	-0.697841051
H	-1.459387105	0.934268069	0.184249014
H	2.330389166	2.975319212	1.548459114
O	-1.190003087	3.828121275	1.956787139
H	-0.505877035	3.299186235	1.550007111
H	-1.008719074	4.732924341	1.741037124
O	-3.025574218	2.041475147	0.714214049
H	-3.827940275	1.806167132	1.160814083
H	-2.632485191	2.767795200	1.195402087
O	-0.983868069	-2.472264179	-1.254036090
H	-0.083274004	-2.746495196	-1.410830102
H	-1.402294103	-3.164752227	-0.759140055
O	4.794143344	3.629327263	2.859884207
H	5.062160365	3.612406260	3.768435272
H	5.343857385	3.002945218	2.399863175
O	5.887928423	1.515965107	1.154570082
H	4.995577357	1.387759102	0.850342060
H	6.439767466	1.571438112	0.386154027
O	1.921151136	-2.582743186	-1.558120113
H	2.348440169	-2.574294183	-2.403329174
H	1.874216136	-1.681979122	-1.253049090

Coord_4

C	2.028658146	2.230510162	0.827392061
N	0.743112054	2.035401145	0.605264042
C	0.538116037	0.903632066	-0.130508011
C	2.684285193	0.964436067	-1.004613072
N	3.010530217	1.536743109	0.245948017
N	1.536777108	0.214155016	-0.703105052
H	3.476385248	0.451755035	-1.528110111
N	-0.683832052	0.426108031	-0.214393014

H	-0.849434061	-0.443556031	-0.692147051
H	-1.456723105	0.933370066	0.184354013
H	2.332827170	2.976346213	1.548099109
O	-1.194016087	3.828737274	1.957938141
H	-0.507673036	3.302709238	1.551087114
H	-1.015367075	4.734484340	1.743966125
O	-3.023205218	2.037881144	0.712382053
H	-3.825671274	1.800889129	1.157943084
H	-2.632369190	2.765154198	1.194023088
O	-0.980256070	-2.463894177	-1.256856091
H	-0.079003004	-2.736898196	-1.412780099
H	-1.399276099	-3.158667228	-0.765680056
O	4.790654346	3.623730261	2.850266204
H	5.061203364	3.611246261	3.758153268
H	5.338973386	2.994991218	2.391700171
O	5.882065425	1.502204106	1.154628085
H	4.990006359	1.362379099	0.854691061
H	6.431496462	1.551578111	0.384021030
O	1.922362137	-2.581041188	-1.544394112
H	2.365844168	-2.575971183	-2.381229171
H	1.885806134	-1.681300119	-1.234213089

Coord_5

C	2.025821147	2.231997160	0.828978058
N	0.742084053	2.041598149	0.605879041
C	0.539843039	0.905960065	-0.127687009
C	2.672989190	0.988567073	-1.019222073
N	3.003046216	1.525423108	0.250475017
N	1.545129113	0.215803017	-0.689890052
H	3.463640247	0.490681033	-1.559216113
N	-0.679556051	0.425581029	-0.211445015
H	-0.842609061	-0.446304033	-0.686417051
H	-1.454316105	0.932696068	0.184250014
H	2.335144167	2.977723212	1.547718112
O	-1.199041085	3.829772276	1.958638142
H	-0.510341037	3.306731239	1.551881113
H	-1.023145076	4.736459341	1.746383126
O	-3.021346219	2.034310145	0.709988050
H	-3.823940277	1.795548127	1.154405085
H	-2.632959191	2.762639198	1.192073086
O	-0.975084071	-2.455928176	-1.259073090
H	-0.072978004	-2.727177195	-1.413928102
H	-1.394368102	-3.153181226	-0.771656054
O	4.788432347	3.616304259	2.840860205
H	5.062389366	3.607963261	3.747787268
H	5.334789383	2.985224215	2.383071174
O	5.875440422	1.486904105	1.153324081

H	4.983434359	1.335769098	0.858687064
H	6.421738460	1.530309112	0.380106028
O	1.925104138	-2.578159188	-1.529835112
H	2.384628172	-2.576426185	-2.357962169
H	1.898303136	-1.679675122	-1.214347087

Coord_6

C	2.022724148	2.233902161	0.830569061
N	0.740681056	2.048421149	0.606533046
C	0.541370038	0.908784067	-0.124773010
C	2.660262192	1.013874070	-1.032981073
N	2.994668213	1.513931108	0.254827019
N	1.553732111	0.218436018	-0.676157050
H	3.449049248	0.531199039	-1.589538112
N	-0.675389050	0.425373030	-0.208535016
H	-0.835686062	-0.448790034	-0.680648050
H	-1.452151104	0.932249067	0.183927015
H	2.337361166	2.979475217	1.547277112
O	-1.205097085	3.831234276	1.958865144
H	-0.513897039	3.311265240	1.552371110
H	-1.032084076	4.738859339	1.748260123
O	-3.019992218	2.030752148	0.707018053
H	-3.822740278	1.790127130	1.150184081
H	-2.634260189	2.760244200	1.189532088
O	-0.968305072	-2.448366175	-1.260630088
H	-0.065155007	-2.717321194	-1.414218102
H	-1.387507102	-3.148290226	-0.776998056
O	4.787471345	3.606964259	2.831689204
H	5.065737365	3.602446260	3.737345267
H	5.331279382	2.973563212	2.373975173
O	5.867996422	1.470004105	1.150606084
H	4.975803358	1.307885093	0.862292062
H	6.410404462	1.507598111	0.374349030
O	1.929426140	-2.574059186	-1.514401108
H	2.404833176	-2.575600187	-2.333491166
H	1.911741137	-1.677049122	-1.193423085

Coord_7

C	2.019376144	2.236247163	0.832139061
N	0.738909053	2.055898148	0.607218045
C	0.542713037	0.912127065	-0.121772009
C	2.646070192	1.040381077	-1.045845076
N	2.985357213	1.502267110	0.258976017
N	1.562603112	0.222107016	-0.661899047
H	3.432555248	0.573372043	-1.619047115
N	-0.671311046	0.425494032	-0.205668013
H	-0.828634061	-0.451007032	-0.674840050

H	-1.450213103	0.932032067	0.183377014
H	2.339500169	2.981632212	1.546735113
O	-1.212205089	3.833132276	1.958592141
H	-0.518356040	3.316330239	1.552535112
H	-1.042215073	4.741690342	1.749566128
O	-3.019139216	2.027194145	0.703454050
H	-3.822062274	1.784604128	1.145263082
H	-2.636276190	2.757961197	1.186381086
O	-0.959874067	-2.441202173	-1.261468088
H	-0.055491003	-2.707314193	-1.413592101
H	-1.378628100	-3.143991227	-0.781632056
O	4.787771346	3.595618260	2.822779203
H	5.071276364	3.594573256	3.726835267
H	5.328421385	2.959924213	2.364407172
O	5.859666421	1.451442107	1.146422081
H	4.967042358	1.278681092	0.865467062
H	6.397389459	1.483408106	0.366687025
O	1.935376140	-2.568703187	-1.498051107
H	2.426498174	-2.573427184	-2.307780168
H	1.926153136	-1.673361122	-1.171413085

Coord_8

C	2.015790143	2.239053162	0.833661060
N	0.736779051	2.064053150	0.607923041
C	0.543884037	0.916014068	-0.118691007
C	2.630371191	1.068115077	-1.057764074
N	2.975072214	1.490432109	0.262890018
N	1.571765112	0.226871019	-0.647109045
H	3.414094244	0.617267047	-1.647711117
N	-0.667299046	0.425956030	-0.202850012
H	-0.821421058	-0.452943033	-0.668994049
H	-1.448485107	0.932047070	0.182589011
H	2.341583170	2.984219217	1.546048114
O	-1.220388090	3.835473277	1.957793142
H	-0.523737037	3.321938238	1.552350112
H	-1.053571074	4.744962341	1.750267123
O	-3.018779217	2.023619145	0.699278048
H	-3.821896277	1.778958130	1.139621084
H	-2.639010190	2.755779198	1.182596087
O	-0.949737068	-2.434433176	-1.261523091
H	-0.043937005	-2.697139194	-1.411988101
H	-1.367659097	-3.140274228	-0.785478058
O	4.789341346	3.582169257	2.814158202
H	5.079043368	3.584213257	3.716262269
H	5.326190385	2.944215211	2.354365171
O	5.850372423	1.431153102	1.140715084
H	4.957079358	1.248112088	0.868173063

H	6.382577460	1.457705105	0.357058025
O	1.943009141	-2.562044185	-1.480739106
H	2.449669178	-2.569837182	-2.280787165
H	1.941574139	-1.668546122	-1.148287081

Coord_9

C	2.011976145	2.242342163	0.835107058
N	0.734299051	2.072916150	0.608637044
C	0.544900042	0.920470068	-0.115536010
C	2.613125188	1.097100078	-1.068685075
N	2.963769215	1.478429104	0.266539018
N	1.581237115	0.232787019	-0.631779045
H	3.393595245	0.662953046	-1.675486123
N	-0.663330048	0.426769032	-0.200085014
H	-0.814011057	-0.454589033	-0.663107047
H	-1.446947106	0.932294068	0.181553015
H	2.343636171	2.987268215	1.545167113
O	-1.229668086	3.838266274	1.956434140
H	-0.530057038	3.328108238	1.551788110
H	-1.066187078	4.748680340	1.750326127
O	-3.018905219	2.020011146	0.694469049
H	-3.822232273	1.773161125	1.133240080
H	-2.642468189	2.753686197	1.178152083
O	-0.937840068	-2.428048176	-1.260729092
H	-0.030441001	-2.686775194	-1.409341103
H	-1.354524098	-3.137131227	-0.788455056
O	4.792196347	3.566512257	2.805852204
H	5.089081368	3.571223257	3.705622266
H	5.324567382	2.926341212	2.343843169
O	5.840027420	1.409070101	1.133428081
H	4.945829356	1.216133087	0.870370064
H	6.365835456	1.430453101	0.345398023
O	1.952377139	-2.554032182	-1.462416105
H	2.474392176	-2.564752186	-2.252468160
H	1.958042141	-1.662533118	-1.124012081

Coord_10

C	2.031688146	2.264279163	0.855384061
N	0.756042055	2.101385150	0.623201045
C	0.572282043	0.942881069	-0.096529005
C	2.625108190	1.140427085	-1.054436078
N	2.976781213	1.482141108	0.294716019
N	1.619009115	0.255062016	-0.594017041
H	3.404056244	0.721336050	-1.673898120
N	-0.632993046	0.446297032	-0.185591013
H	-0.778891056	-0.438519031	-0.643937046
H	-1.420302100	0.952789066	0.187484012

H	2.367134170	3.010282218	1.562671111
O	-1.219495088	3.865492280	1.955738140
H	-0.515543040	3.357187242	1.556284111
H	-1.057741076	4.776184343	1.749504124
O	-2.995314217	2.039110148	0.686934052
H	-3.800974275	1.791770130	1.121160080
H	-2.623802191	2.775198199	1.170816083
O	-0.896030065	-2.405912173	-1.241652088
H	0.013506000	-2.661313191	-1.383723098
H	-1.313764093	-3.116905226	-0.773223054
O	4.812966348	3.568537259	2.825701203
H	5.114213367	3.577260259	3.724006270
H	5.341484385	2.924589212	2.364425169
O	5.850140421	1.400177103	1.161846084
H	4.955701359	1.198042088	0.906002066
H	6.372034460	1.414289101	0.371180025
O	1.992265145	-2.531771182	-1.412996104
H	2.532767184	-2.547615183	-2.190398156
H	2.003736146	-1.641610116	-1.070561077

LIIC path connecting S₁/S₀ and S0-MIN

Coord_1

C	2.031688146	2.264279163	0.855384061
N	0.756042055	2.101385150	0.623201045
C	0.572282043	0.942881069	-0.096529005
C	2.625108190	1.140427085	-1.054436078
N	2.976781213	1.482141108	0.294716019
N	1.619009115	0.255062016	-0.594017041
H	3.404056244	0.721336050	-1.673898120
N	-0.632993046	0.446297032	-0.185591013
H	-0.778891056	-0.438519031	-0.643937046
H	-1.420302100	0.952789066	0.187484012
H	2.367134170	3.010282218	1.562671111
O	-1.219495088	3.865492280	1.955738140
H	-0.515543040	3.357187242	1.556284111
H	-1.057741076	4.776184343	1.749504124
O	-2.995314217	2.039110148	0.686934052
H	-3.800974275	1.791770130	1.121160080
H	-2.623802191	2.775198199	1.170816083
O	-0.896030065	-2.405912173	-1.241652088
H	0.013506000	-2.661313191	-1.383723098
H	-1.313764093	-3.116905226	-0.773223054
O	4.812966348	3.568537259	2.825701203
H	5.114213367	3.577260259	3.724006270
H	5.341484385	2.924589212	2.364425169
O	5.850140421	1.400177103	1.161846084
H	4.955701359	1.198042088	0.906002066

H	6.372034460	1.414289101	0.371180025
O	1.992265145	-2.531771182	-1.412996104
H	2.532767184	-2.547615183	-2.190398156
H	2.003736146	-1.641610116	-1.070561077

Coord_2

C	2.039210146	2.241906163	0.835436058
N	0.763860056	2.070970148	0.605297041
C	0.559429042	0.933004065	-0.131913008
C	2.659155190	1.044187074	-1.033839076
N	2.999187218	1.482991109	0.279687020
N	1.579533111	0.224193017	-0.653091045
H	3.440262249	0.602296046	-1.634399119
N	-0.660698047	0.467681032	-0.238112019
H	-0.818988059	-0.413801030	-0.697505050
H	-1.433229101	0.975920071	0.160958013
H	2.366082171	2.992370214	1.541609110
O	-1.156831082	3.849542280	1.995930142
H	-0.470788032	3.334604238	1.575233112
H	-0.982658069	4.760079342	1.799281129
O	-2.989642215	2.074509148	0.727681054
H	-3.788939271	1.827581131	1.173654087
H	-2.598271188	2.794531203	1.219570088
O	-0.906530063	-2.428988175	-1.240884088
H	0.001353000	-2.687246194	-1.385602101
H	-1.324951096	-3.138311224	-0.770428056
O	4.725694341	3.589980257	2.804832204
H	4.977229359	3.591415259	3.718301268
H	5.281450380	2.952341214	2.367455169
O	5.858841423	1.442970106	1.175842087
H	4.981286359	1.255955088	0.864699062
H	6.422420464	1.470985104	0.412046029
O	1.989466141	-2.534976181	-1.451757105
H	2.496797180	-2.549269185	-2.244559161
H	1.971983141	-1.644728119	-1.122730080

Coord_3

C	2.043772147	2.226964161	0.817150057
N	0.768765053	2.046607145	0.588770042
C	0.547909039	0.926427064	-0.162147011
C	2.686435193	0.954500071	-1.001791070
N	3.016552217	1.487455106	0.267718020
N	1.546393111	0.201640017	-0.701404049
H	3.469803252	0.490116036	-1.582041115
N	-0.684618049	0.489091035	-0.286436019
H	-0.852018060	-0.390968026	-0.744066054
H	-1.445235106	0.996545071	0.134415011

H	2.361089172	2.984295217	1.519988108
O	-1.109949079	3.835922279	2.025764144
H	-0.438804030	3.316415241	1.587819117
H	-0.926541065	4.746114344	1.835967130
O	-2.987778214	2.101114153	0.760093055
H	-3.780892274	1.852423135	1.215933090
H	-2.581118188	2.807928203	1.258257088
O	-0.917029067	-2.452063176	-1.240115088
H	-0.010801000	-2.713178197	-1.387481098
H	-1.336137094	-3.159716227	-0.767632053
O	4.670468334	3.604642261	2.796899202
H	4.885809353	3.593379258	3.719460267
H	5.243054379	2.972756216	2.373126171
O	5.864319424	1.481519107	1.179585085
H	4.999194358	1.315560094	0.828184059
H	6.456984464	1.525766110	0.437409029
O	1.986666142	-2.538180185	-1.490519105
H	2.460827177	-2.550922186	-2.298720167
H	1.940230140	-1.647846121	-1.174898082

Coord_4

C	2.046679150	2.217726160	0.800811059
N	0.771929057	2.027275146	0.573927044
C	0.537965036	0.922521064	-0.187878011
C	2.707573194	0.871464064	-0.959152068
N	3.030243218	1.494006108	0.258396018
N	1.519570111	0.185789015	-0.740264053
H	3.493019252	0.385100027	-1.518146111
N	-0.704914050	0.510438035	-0.331454022
H	-0.878849061	-0.369774028	-0.785070057
H	-1.456233103	1.015129072	0.107606008
H	2.353817171	2.983583215	1.498610109
O	-1.076521079	3.824751273	2.047732149
H	-0.417505032	3.302271238	1.595906115
H	-0.886576065	4.734608342	1.862745134
O	-2.989356216	2.120649155	0.785132056
H	-3.776587274	1.868384137	1.249054087
H	-2.571285186	2.816734205	1.288494091
O	-0.927529065	-2.475138178	-1.239347087
H	-0.022954000	-2.739110200	-1.389360101
H	-1.347323096	-3.181121229	-0.764837055
O	4.639086335	3.613367261	2.798525200
H	4.829922346	3.586635259	3.726103267
H	5.221449374	2.987028217	2.379905170
O	5.868634425	1.515890112	1.174095082
H	5.011200363	1.374308098	0.795165055
H	6.480336469	1.578329111	0.448406031

O	1.983866144	-2.541383184	-1.529279111
H	2.424856174	-2.552575182	-2.352880167
H	1.908477140	-1.650963118	-1.227067090

Coord_5

C	2.048711148	2.213043158	0.786607058
N	0.774033055	2.012247147	0.560913041
C	0.529658038	0.920877064	-0.209629016
C	2.722943194	0.795367058	-0.906728066
N	3.041257217	1.501744108	0.251509019
N	1.498892108	0.175561014	-0.770662053
H	3.510093252	0.287692022	-1.443900103
N	-0.721780051	0.531671039	-0.373836029
H	-0.900182064	-0.350010025	-0.821552061
H	-1.466223107	1.031974075	0.080340007
H	2.345239171	2.988543214	1.478050107
O	-1.054978077	3.815952272	2.063589147
H	-0.405503028	3.291799238	1.600774117
H	-0.860845064	4.725598343	1.881870134
O	-2.994168215	2.134237156	0.803517060
H	-3.775879272	1.876835135	1.273830092
H	-2.568080187	2.821773205	1.311454097
O	-0.938029069	-2.498213179	-1.238578087
H	-0.035108000	-2.765042197	-1.391239098
H	-1.358509099	-3.202526232	-0.762041057
O	4.626572335	3.616720261	2.806970202
H	4.802864344	3.573254255	3.736746270
H	5.213633373	2.995938218	2.386669172
O	5.872990421	1.546222112	1.160530084
H	5.018682363	1.430783101	0.764905054
H	6.495665469	1.628392115	0.446686030
O	1.981066140	-2.544587183	-1.568040112
H	2.388886170	-2.554228184	-2.407041173
H	1.876724134	-1.654081120	-1.279235093

Coord_6

C	2.050240148	2.212099159	0.774719054
N	0.775378054	2.000964147	0.549774039
C	0.522893036	0.921190067	-0.227846017
C	2.732736196	0.726581054	-0.845194060
N	3.050268221	1.510138109	0.247052019
N	1.484080108	0.170197014	-0.793328059
H	3.521094254	0.198378015	-1.360304100
N	-0.735465051	0.552732040	-0.414153028
H	-0.916636068	-0.331518026	-0.854335062
H	-1.475310107	1.047257074	0.052384002
H	2.335800167	2.997957214	1.458813107

O	-1.044343075	3.809301276	2.074540147
H	-0.401955027	3.284586235	1.603284115
H	-0.848107059	4.718927339	1.894925138
O	-3.002175217	2.142598157	0.815670060
H	-3.778768273	1.878665135	1.290742094
H	-2.571129185	2.823513204	1.327895094
O	-0.948528067	-2.521288181	-1.237810087
H	-0.047261005	-2.790974200	-1.393118101
H	-1.369696096	-3.223931230	-0.759245054
O	4.630394334	3.615248259	2.820349205
H	4.800865345	3.554655257	3.750209270
H	5.218082378	3.000125216	2.392702173
O	5.878063421	1.572704116	1.139899082
H	5.022635359	1.484241105	0.737165054
H	6.504955467	1.675676119	0.433689029
O	1.978266142	-2.547791182	-1.606801117
H	2.352915167	-2.555882186	-2.461201178
H	1.844971134	-1.657199117	-1.331404095

Coord_7

C	2.051273149	2.214237162	0.765438058
N	0.775934055	1.992924145	0.540533038
C	0.517428038	0.923193066	-0.242921018
C	2.736986199	0.665489048	-0.774998057
N	3.057656218	1.518832110	0.245317016
N	1.474774108	0.169144014	-0.808744056
H	3.525976253	0.117618010	-1.268078089
N	-0.746290054	0.573557043	-0.452995035
H	-0.928810066	-0.314174025	-0.884211066
H	-1.483725105	1.061069077	0.023358000
H	2.325478168	3.010839219	1.441497104
O	-1.044172077	3.804430274	2.081370148
H	-0.406501030	3.280148237	1.603991117
H	-0.847682061	4.714265340	1.903019137
O	-3.013532218	2.146190154	0.821616059
H	-3.785465270	1.874453133	1.299797095
H	-2.580373186	2.822182201	1.338134097
O	-0.959028071	-2.544363182	-1.237041086
H	-0.059415005	-2.816906203	-1.394997098
H	-1.380882099	-3.245336232	-0.756450056
O	4.650054332	3.609551258	2.837726206
H	4.823046349	3.532039253	3.765817274
H	5.234604376	3.000256214	2.397647171
O	5.884224426	1.595663116	1.112920081
H	5.023666361	1.534288112	0.712310053
H	6.509048468	1.720019124	0.410107029
O	1.975466143	-2.550995186	-1.645563118

H	2.316945169	-2.557535182	-2.515362179
H	1.813218128	-1.660316119	-1.383572098

Coord_8

C	2.051334148	2.218742159	0.759439056
N	0.775231054	1.987564146	0.533283040
C	0.512802039	0.926588067	-0.255216017
C	2.735514197	0.612392044	-0.696091051
N	3.063410222	1.527425112	0.247216016
N	1.470515105	0.171962010	-0.817089059
H	3.524538256	0.045750003	-1.167380082
N	-0.754705052	0.594089041	-0.491180036
H	-0.937348066	-0.297826020	-0.912249067
H	-1.491919107	1.073460080	-0.007526001
H	2.313628164	3.026157218	1.427154104
O	-1.054750076	3.800742273	2.084482149
H	-0.419419029	3.277824233	1.603219117
H	-0.859575060	4.711030337	1.906922137
O	-3.028750218	2.145315154	0.820610062
H	-3.796634276	1.864592132	1.300047094
H	-2.596248186	2.817811202	1.341797094
O	-0.969527070	-2.567438184	-1.236273092
H	-0.071568006	-2.842838206	-1.396876101
H	-1.392068102	-3.266741235	-0.753654053
O	4.687603337	3.600324259	2.859506205
H	4.872840351	3.506829255	3.783709275
H	5.264846380	2.997318217	2.401515171
O	5.891705426	1.615895118	1.079780075
H	5.021854363	1.580524112	0.691836048
H	6.507122469	1.761703125	0.374865025
O	1.972666144	-2.554199185	-1.684324124
H	2.280975166	-2.559188183	-2.569523184
H	1.781465128	-1.663434122	-1.435741106

Coord_9

C	2.048792149	2.224226161	0.758840053
N	0.771775056	1.983874145	0.528548036
C	0.508000036	0.930889066	-0.265091020
C	2.727615195	0.567121041	-0.606909042
N	3.066615221	1.534822110	0.255700018
N	1.470582104	0.178141012	-0.817923058
H	3.516202254	-0.017416001	-1.056542077
N	-0.761514055	0.614386042	-0.530508040
H	-0.943111070	-0.282079023	-0.940864067
H	-1.500971108	1.084549079	-0.042491002
H	2.298093166	3.042026217	1.418657100
O	-1.078194078	3.796993275	2.083712149

H	-0.442562030	3.276357238	1.601080113
H	-0.885352062	4.707994341	1.907193139
O	-3.049419220	2.140292156	0.809553056
H	-3.814397274	1.849473131	1.287545091
H	-2.620576189	2.810230204	1.336605098
O	-0.980027068	-2.590514185	-1.235504091
H	-0.083721006	-2.868770204	-1.398755103
H	-1.403254099	-3.288146238	-0.750859055
O	4.751160340	3.588404256	2.889493209
H	4.965395357	3.481839251	3.805936275
H	5.315098385	2.993638217	2.404949171
O	5.900816424	1.636085120	1.039175077
H	5.016026359	1.621549118	0.680803046
H	6.493522465	1.802818128	0.321192021
O	1.969866141	-2.557403184	-1.723085124
H	2.245004162	-2.560841185	-2.623683190
H	1.749712128	-1.666551119	-1.487909108

Coord_10

C	2.010404145	2.225413158	0.765495055
N	0.733465052	1.970661140	0.527942038
C	0.473481037	0.886914066	-0.219420018
C	2.683538196	0.459482034	-0.411087028
N	3.035677217	1.507145108	0.318932022
N	1.446775102	0.107636007	-0.709087052
H	3.471976249	-0.166874013	-0.800625058
N	-0.794624056	0.576531040	-0.514996040
H	-0.974985073	-0.343057027	-0.869526064
H	-1.541119113	1.064285077	-0.057112005
H	2.243360162	3.084142222	1.377352101
O	-1.151952084	3.867401276	1.967531141
H	-0.511431036	3.323101237	1.519413109
H	-0.955890071	4.768363342	1.748159125
O	-3.108885222	2.151434157	0.743146053
H	-3.878275281	1.877573136	1.223994089
H	-2.688481193	2.843955204	1.246873089
O	-0.991563074	-2.610662186	-1.235090089
H	-0.096889005	-2.891674207	-1.401037101
H	-1.415368104	-3.306666240	-0.748383056
O	4.834936348	3.676631264	2.879494209
H	5.122060367	3.616109262	3.780013273
H	5.373438388	3.071854219	2.378706171
O	5.880408423	1.667978119	1.026812073
H	4.971025359	1.635707118	0.740742054
H	6.411359463	1.811739131	0.255726017
O	1.965991140	-2.557345186	-1.762375127
H	2.207905159	-2.559217182	-2.678387195

H 1.716794122 -1.666433123 -1.540605113

LIIC path connecting S1-MIN and T1-MIN

Coord_1

C	2.035513145	2.228362162	0.822884058
N	0.743864051	2.020331145	0.603730042
C	0.531622037	0.899398066	-0.138366007
C	2.709915195	0.898875065	-0.956046067
N	3.027953219	1.569674110	0.231588015
N	1.513038111	0.214646013	-0.739703051
H	3.504027251	0.343978023	-1.430275101
N	-0.697489048	0.429476032	-0.223432017
H	-0.869588062	-0.433855032	-0.709117051
H	-1.465534107	0.936715069	0.183437013
H	2.325074168	2.974204215	1.549250112
O	-1.184937083	3.828100277	1.953210139
H	-0.504848034	3.293568236	1.547056112
H	-0.998707073	4.731003338	1.733732123
O	-3.031856219	2.048767146	0.716246053
H	-3.834117276	1.816593131	1.164605082
H	-2.634817190	2.773471197	1.196510089
O	-0.986562068	-2.490214178	-1.246802089
H	-0.086706004	-2.765346199	-1.404729101
H	-1.402884099	-3.178712229	-0.744633052
O	4.804972348	3.635352264	2.879658206
H	5.070462368	3.608760260	3.788691272
H	5.355823385	3.013705217	2.414794175
O	5.897555422	1.539101112	1.150562083
H	5.003932362	1.435003104	0.840745060
H	6.452144466	1.607066113	0.385298030
O	1.923135138	-2.582725188	-1.583203114
H	2.317628168	-2.567490186	-2.444150177
H	1.853648133	-1.680706123	-1.287718095

Coord_2

C	2.050425148	2.209218159	0.834670058
N	0.750311055	2.008410147	0.595167044
C	0.534138037	0.870903062	-0.134194011
C	2.709376196	0.886278064	-0.948953071
N	3.039621217	1.570393114	0.225763017
N	1.506973110	0.206375015	-0.757705053
H	3.501404251	0.342724027	-1.438762104
N	-0.694055052	0.383691029	-0.175619011
H	-0.864896064	-0.478914036	-0.662899049
H	-1.457980108	0.912811064	0.209970013
H	2.333712166	2.937547212	1.580301111
O	-1.159218084	3.836185274	1.944807143

H	-0.480973033	3.310512237	1.525822107
H	-0.969462071	4.744343341	1.751299125
O	-3.023671217	2.065795149	0.709972053
H	-3.833160275	1.844412132	1.150793085
H	-2.624919189	2.789134198	1.190248085
O	-0.999046074	-2.487914178	-1.254244088
H	-0.099798008	-2.761758198	-1.417328103
H	-1.413414101	-3.180711228	-0.756405055
O	4.772411341	3.654173262	2.878284208
H	5.039751365	3.638937259	3.787043271
H	5.332462384	3.037580218	2.417485174
O	5.896542423	1.565120112	1.164693084
H	5.009897359	1.459568105	0.836421058
H	6.468203466	1.622866118	0.410857031
O	1.910659139	-2.583965188	-1.610533113
H	2.295658167	-2.578505185	-2.476135180
H	1.841325134	-1.678098121	-1.326991096

Coord_3

C	2.066421150	2.191063157	0.846635062
N	0.757829055	1.999240145	0.586590044
C	0.537083041	0.845213062	-0.129199012
C	2.708098196	0.875387061	-0.941901070
N	3.051175221	1.571878112	0.219846016
N	1.500309107	0.200540016	-0.774447057
H	3.497325252	0.343062023	-1.447544102
N	-0.689036050	0.342250027	-0.126192010
H	-0.860257064	-0.519596040	-0.614547044
H	-1.449874107	0.891282064	0.236311017
H	2.343663170	2.901016207	1.611337114
O	-1.140624081	3.847101275	1.936010137
H	-0.462603031	3.331644237	1.505686109
H	-0.948273068	4.760004342	1.768881129
O	-3.016787219	2.081986152	0.700024050
H	-3.833663274	1.869830135	1.131723082
H	-2.618638189	2.804765200	1.181012085
O	-1.009759072	-2.492498181	-1.257910091
H	-0.110496009	-2.761820201	-1.427870102
H	-1.419388100	-3.191921229	-0.765466056
O	4.745426339	3.668572265	2.878370210
H	5.015769359	3.663367262	3.786359273
H	5.313142382	3.056986222	2.420066172
O	5.895763427	1.587748112	1.176156085
H	5.015698359	1.482321107	0.830868062
H	6.483099467	1.635966118	0.433492033
O	1.899632138	-2.581913187	-1.637878120
H	2.273665164	-2.583195188	-2.508468179

H 1.827573130 -1.673167120 -1.364117097

Coord_4

C 2.083612150 2.173604155 0.858857062
N 0.766587055 1.992482144 0.578062040
C 0.540612039 0.822002057 -0.123265008
C 2.706231195 0.866126063 -0.934897065
N 3.062770219 1.574012115 0.213865017
N 1.493200108 0.196896017 -0.789923057
H 3.491967253 0.345045024 -1.456694106
N -0.682277049 0.304907020 -0.074965006
H -0.855571062 -0.556097041 -0.563937040
H -1.441061104 0.871812062 0.262781019
H 2.354887167 2.864281204 1.642488117
O -1.129075079 3.861022277 1.926425139
H -0.449675035 3.357140241 1.486201109
H -0.935426067 4.778170346 1.785788130
O -3.011160218 2.096817149 0.686850050
H -3.835444278 1.892235134 1.108065081
H -2.615935188 2.820024200 1.168971085
O -1.018784073 -2.502581178 -1.258041089
H -0.119104008 -2.764681198 -1.436480102
H -1.421301102 -3.210552232 -0.772020054
O 4.723518338 3.678683265 2.879789209
H 4.997802362 3.682227266 3.786609272
H 5.297579379 3.072069223 2.422565175
O 5.895478422 1.607062118 1.185108086
H 5.021625361 1.503283109 0.823970057
H 6.497293467 1.646414120 0.453388034
O 1.889795135 -2.576881188 -1.665289121
H 2.251501162 -2.582304186 -2.541171185
H 1.812629133 -1.666104123 -1.399275099

Coord_5

C 2.102090152 2.156589153 0.871439060
N 0.776737055 1.987864142 0.569685042
C 0.544832037 0.801020057 -0.116240006
C 2.703864196 0.858469064 -0.927928065
N 3.074511223 1.576723111 0.207865014
N 1.485726109 0.195272014 -0.804100060
H 3.485419251 0.348774025 -1.466272103
N -0.673670049 0.271543019 -0.021712000
H -0.850848059 -0.588467041 -0.510905039
H -1.431417103 0.854217061 0.289739022
H 2.367340168 2.827037201 1.673897120
O -1.124431083 3.878183279 1.915589139
H -0.442130031 3.387208245 1.466833105

H	-0.931085068	4.799106344	1.801239127
O	-3.006747219	2.109913154	0.670929049
H	-3.838315276	1.911185136	1.080544080
H	-2.616737188	2.834692205	1.154301086
O	-1.026096075	-2.517321182	-1.254891092
H	-0.125777008	-2.769812201	-1.443327105
H	-1.419374103	-3.235467235	-0.776326054
O	4.706223338	3.684537267	2.882432206
H	4.985155360	3.695529268	3.787778272
H	5.285493379	3.082871223	2.425019176
O	5.895869426	1.623084118	1.191688088
H	5.027910362	1.522489111	0.815596060
H	6.511173469	1.654235121	0.470761034
O	1.880945138	-2.569043184	-1.692865124
H	2.229006160	-2.576300183	-2.574304185
H	1.796605127	-1.657020118	-1.432637105

Coord_6

C	2.121940151	2.139810155	0.884493064
N	0.788427057	1.985167142	0.561588038
C	0.549826042	0.782081058	-0.107945010
C	2.701033193	0.852432061	-0.920971067
N	3.086469221	1.579981113	0.201894017
N	1.477908108	0.195549012	-0.816919061
H	3.477703249	0.354393025	-1.476331107
N	-0.663131045	0.242142016	0.033841001
H	-0.846191061	-0.616630044	-0.455227030
H	-1.420829102	0.838425062	0.317592023
H	2.380993169	2.789006201	1.705710124
O	-1.126477083	3.898863282	1.902974136
H	-0.439899030	3.422072247	1.446961103
H	-0.935274067	4.823127345	1.814357129
O	-3.003487217	2.121021150	0.652784048
H	-3.842068275	1.926376137	1.049954074
H	-2.620925187	2.848648207	1.137190081
O	-1.031588072	-2.536309184	-1.248723092
H	-0.130558008	-2.776938203	-1.448614104
H	-1.413608103	-3.266048235	-0.778698054
O	4.693058339	3.686075263	2.886180210
H	4.977066356	3.703147267	3.789858272
H	5.276567381	3.089346220	2.427469177
O	5.897046422	1.635789119	1.196033088
H	5.034751365	1.539997109	0.805579057
H	6.525093471	1.659430118	0.485878035
O	1.872923134	-2.558455183	-1.720751125
H	2.205999158	-2.565420182	-2.607972187
H	1.779507130	-1.645966118	-1.464356106

Coord_7

C	2.143256152	2.123090154	0.898136063
N	0.801806060	1.984217142	0.553924038
C	0.555658041	0.765044053	-0.098167005
C	2.697729195	0.848069059	-0.913996066
N	3.098690226	1.583797116	0.195994013
N	1.469716105	0.197656016	-0.828293059
H	3.468777251	0.362090025	-1.486928109
N	-0.650594048	0.216788017	0.092018007
H	-0.841786063	-0.640391045	-0.396598028
H	-1.409186102	0.824470060	0.346806026
H	2.395835173	2.749937198	1.738057126
O	-1.134889081	3.923367284	1.887991138
H	-0.442862031	3.461950251	1.425872103
H	-0.947830067	4.850583347	1.824180130
O	-3.001284215	2.129997155	0.633002048
H	-3.846455277	1.937648142	1.017197071
H	-2.628310189	2.861860208	1.117865078
O	-1.035068074	-2.559521184	-1.239810091
H	-0.133388010	-2.786014201	-1.452586103
H	-1.403799099	-3.302151237	-0.779514056
O	4.683434336	3.683163264	2.890869207
H	4.972577356	3.704811265	3.792823273
H	5.270379378	3.091362221	2.429943176
O	5.899041426	1.645103120	1.198282086
H	5.042320362	1.555896113	0.793690058
H	6.539385469	1.661984118	0.499109038
O	1.865598135	-2.545070184	-1.749148125
H	2.182275158	-2.549682181	-2.642328189
H	1.761247128	-1.632942119	-1.494564110

Coord_8

C	2.166155154	2.106289152	0.912464066
N	0.817045058	1.984878142	0.546864041
C	0.562383042	0.749813052	-0.086654008
C	2.693901196	0.845474063	-0.906986066
N	3.111202225	1.588230113	0.190174016
N	1.461072106	0.201548014	-0.838103058
H	3.458528247	0.372101026	-1.498139110
N	-0.635993047	0.195676015	0.153225013
H	-0.837908062	-0.659424047	-0.334586027
H	-1.396359100	0.812516058	0.377943027
H	2.411905174	2.709606197	1.771030128
O	-1.149164082	3.952047284	1.870000133
H	-0.450786032	3.507060251	1.402763102
H	-0.968318069	4.881874349	1.829657131

O	-2.999973215	2.136849154	0.612292045
H	-3.851156276	1.945029138	0.983350068
H	-2.638577191	2.874420208	1.096633079
O	-1.036233074	-2.587372185	-1.228436088
H	-0.134091012	-2.797248200	-1.455553105
H	-1.389496099	-3.344158242	-0.779258056
O	4.676492335	3.675579265	2.896210209
H	4.970295359	3.700093269	3.796589275
H	5.266289377	3.088688220	2.432435177
O	5.901785427	1.650883117	1.198603085
H	5.050783361	1.570319114	0.779581055
H	6.554407472	1.661852120	0.511016039
O	1.858867133	-2.528738182	-1.778337129
H	2.157585155	-2.528859183	-2.677601192
H	1.741635126	-1.617914115	-1.523350109

Coord_9

C	2.190828160	2.089319152	0.927534066
N	0.834372062	1.987051145	0.540604038
C	0.570069040	0.736305051	-0.073049003
C	2.689451196	0.844735062	-0.899913067
N	3.124039224	1.593378113	0.184392014
N	1.451855103	0.207155017	-0.846123062
H	3.446763250	0.384645030	-1.510037110
N	-0.619243042	0.179136013	0.218066017
H	-0.834924058	-0.673258048	-0.268452021
H	-1.382156099	0.802900060	0.411774032
H	2.429349174	2.667870194	1.804637128
O	-1.168458085	3.985396288	1.848296135
H	-0.463186031	3.557668255	1.376711098
H	-0.995846070	4.917536355	1.829597133
O	-2.999249216	2.141824156	0.591589043
H	-3.855707279	1.948874140	0.949803067
H	-2.651190189	2.886649209	1.073948076
O	-1.034623073	-2.620965188	-1.214865088
H	-0.132371011	-2.811251204	-1.458009106
H	-1.369883097	-3.393379246	-0.778745056
O	4.670805335	3.663045263	2.901611209
H	4.967916358	3.688419264	3.800884273
H	5.263194379	3.080989220	2.434839177
O	5.905046423	1.652881121	1.197258086
H	5.060332364	1.583459114	0.762703053
H	6.570596475	1.658925119	0.522578038
O	1.852578131	-2.509178182	-1.808889130
H	2.131561155	-2.502107178	-2.714300195
H	1.720355125	-1.600906115	-1.550616109

Coord_10

C	2.407829171	2.029857145	0.980960071
N	1.038863074	1.949059140	0.591667044
C	0.752902055	0.679947049	0.010798999
C	2.847250206	0.791590055	-0.853764064
N	3.316175238	1.550415112	0.206815016
N	1.604170117	0.163116014	-0.792671059
H	3.586759261	0.340098027	-1.490943109
N	-0.422672030	0.127998007	0.374079027
H	-0.664090047	-0.723259054	-0.102092008
H	-1.185118088	0.759254055	0.542419037
H	2.651867191	2.587215189	1.869896134
O	-0.984758071	3.994929289	1.893237137
H	-0.279822018	3.580436259	1.410837103
H	-0.820116059	4.928731354	1.885988133
O	-2.812620201	2.113047153	0.678807048
H	-3.669201266	1.921617140	1.037650073
H	-2.471278179	2.868816206	1.148115083
O	-0.877262063	-2.707545195	-1.085605078
H	0.021603000	-2.880417205	-1.352890099
H	-1.188104087	-3.489250251	-0.648025046
O	4.883151354	3.608940260	2.901336211
H	5.192565372	3.637391263	3.796362273
H	5.470909392	3.027340220	2.427970175
O	6.100546439	1.601362117	1.185884088
H	5.257464378	1.545553111	0.744722054
H	6.772052487	1.598207115	0.517874039
O	1.992320142	-2.547043185	-1.759953126
H	2.236736159	-2.546465185	-2.674907193
H	1.845557134	-1.638177116	-1.509195109

LIIC path connecting T1-MIN and T₁/S₀

Coord_1

C	2.407829171	2.029857145	0.980960071
N	1.038863074	1.949059140	0.591667044
C	0.752902055	0.679947049	0.010798999
C	2.847250206	0.791590055	-0.853764064
N	3.316175238	1.550415112	0.206815016
N	1.604170117	0.163116014	-0.792671059
H	3.586759261	0.340098027	-1.490943109
N	-0.422672030	0.127998007	0.374079027
H	-0.664090047	-0.723259054	-0.102092008
H	-1.185118088	0.759254055	0.542419037
H	2.651867191	2.587215189	1.869896134
O	-0.984758071	3.994929289	1.893237137
H	-0.279822018	3.580436259	1.410837103
H	-0.820116059	4.928731354	1.885988133

O	-2.812620201	2.113047153	0.678807048
H	-3.669201266	1.921617140	1.037650073
H	-2.471278179	2.868816206	1.148115083
O	-0.877262063	-2.707545195	-1.085605078
H	0.021603000	-2.880417205	-1.352890099
H	-1.188104087	-3.489250251	-0.648025046
O	4.883151354	3.608940260	2.901336211
H	5.192565372	3.637391263	3.796362273
H	5.470909392	3.027340220	2.427970175
O	6.100546439	1.601362117	1.185884088
H	5.257464378	1.545553111	0.744722054
H	6.772052487	1.598207115	0.517874039
O	1.992320142	-2.547043185	-1.759953126
H	2.236736159	-2.546465185	-2.674907193
H	1.845557134	-1.638177116	-1.509195109

Coord_2

C	2.379854173	2.058386149	0.971326071
N	1.025384072	1.954285141	0.594569042
C	0.752378053	0.693929050	-0.007150000
C	2.848972207	0.816681058	-0.875954064
N	3.304470239	1.540784112	0.227994017
N	1.619464117	0.162879011	-0.790026056
H	3.599272260	0.367019025	-1.503076106
N	-0.428953031	0.143218012	0.320587024
H	-0.666010050	-0.711963051	-0.151315012
H	-1.190829085	0.766265056	0.521184037
H	2.631718191	2.647234192	1.837617131
O	-0.978907070	3.968421287	1.916854138
H	-0.279322020	3.543640253	1.434764101
H	-0.813986059	4.901771355	1.890319137
O	-2.812485203	2.099681152	0.701548049
H	-3.664469263	1.905532136	1.069760078
H	-2.465102178	2.852354205	1.171956084
O	-0.878009061	-2.678095195	-1.095496079
H	0.021948002	-2.864625206	-1.350383095
H	-1.200296087	-3.447785250	-0.644966047
O	4.888989354	3.625321259	2.867143206
H	5.171861370	3.653206265	3.770931269
H	5.474923392	3.024387215	2.416269172
O	6.101513441	1.571308114	1.202266087
H	5.260606379	1.497625109	0.760417054
H	6.773703488	1.558424114	0.534623039
O	1.995372145	-2.559549183	-1.730222122
H	2.265997164	-2.572196186	-2.637682188
H	1.865637135	-1.645364121	-1.488480106

Coord_3

C	2.350497171	2.086352150	0.962936072
N	1.010893072	1.961536139	0.598182042
C	0.751584054	0.709785052	-0.023582001
C	2.849045207	0.845166061	-0.895698064
N	3.289568238	1.530720108	0.251393018
N	1.634958120	0.165141011	-0.784881056
H	3.610171258	0.397825031	-1.512692108
N	-0.434727032	0.160878012	0.268358018
H	-0.666517049	-0.698234050	-0.199600012
H	-1.196250088	0.774155057	0.499839038
H	2.609201186	2.704974192	1.806452131
O	-0.977686073	3.943468283	1.938099138
H	-0.282616021	3.508895253	1.457356107
H	-0.813499057	4.876117350	1.891726135
O	-2.813155205	2.084693148	0.721173053
H	-3.660547265	1.886783138	1.097878080
H	-2.461254176	2.834989206	1.192584086
O	-0.875560065	-2.650095189	-1.104046080
H	0.025390004	-2.848751207	-1.346792099
H	-1.208396087	-3.408364244	-0.641872048
O	4.901920350	3.636756261	2.835010204
H	5.163011373	3.665454263	3.745309269
H	5.483330394	3.017452215	2.403632171
O	6.100876439	1.538226112	1.214698085
H	5.259741381	1.445439104	0.777883058
H	6.769650488	1.515121111	0.543395040
O	2.000355143	-2.568536184	-1.698959124
H	2.297003167	-2.593132189	-2.597993185
H	1.886708137	-1.650043117	-1.464413104

Coord_4

C	2.320121169	2.114179153	0.955374071
N	0.995561071	1.971088143	0.602382042
C	0.750714055	0.727720055	-0.038522003
C	2.847455204	0.877337064	-0.913216064
N	3.271554235	1.520368110	0.276423017
N	1.650853118	0.170143011	-0.777205055
H	3.619392262	0.432828032	-1.520076110
N	-0.439727032	0.181084015	0.217428015
H	-0.665316050	-0.682029050	-0.246779016
H	-1.201204087	0.783060057	0.478421033
H	2.585035185	2.761109199	1.775872127
O	-0.981074072	3.920372284	1.956968138
H	-0.289634023	3.476510251	1.478630107
H	-0.818625060	4.852032350	1.890192135
O	-2.814559202	2.068250150	0.737712054

H	-3.657369265	1.865543132	1.122061083
H	-2.459693177	2.816937203	1.210025085
O	-0.869550062	-2.623508191	-1.110442081
H	0.032347002	-2.832756205	-1.341385098
H	-1.211942088	-3.370973241	-0.637694045
O	4.920138357	3.641561264	2.805129200
H	5.164304370	3.671879263	3.720064270
H	5.494927393	3.005286218	2.389957172
O	6.098441441	1.501746109	1.222338087
H	5.254796378	1.388976098	0.796209058
H	6.759742485	1.469210106	0.543553037
O	2.007739145	-2.573916186	-1.665766121
H	2.330158169	-2.609272185	-2.555509184
H	1.909106136	-1.651993119	-1.436769101

Coord_5

C	2.289083167	2.142198152	0.948305067
N	0.979572071	1.983182145	0.607094043
C	0.749954056	0.747922052	-0.051968005
C	2.844179205	0.913421068	-0.928625066
N	3.250507236	1.509783110	0.302605020
N	1.667360119	0.178104012	-0.766904053
H	3.626881263	0.472268035	-1.525392108
N	-0.443715033	0.203935016	0.167798010
H	-0.662122047	-0.663301049	-0.292741023
H	-1.205523088	0.793114059	0.456912031
H	2.559925185	2.816172203	1.745392126
O	-0.989078073	3.899388279	1.973451142
H	-0.300320022	3.446752248	1.498621105
H	-0.829334062	4.829722349	1.885716136
O	-2.816609203	2.050531148	0.751093052
H	-3.654859261	1.842007133	1.142225081
H	-2.460370180	2.798413200	1.224223091
O	-0.859637064	-2.598318185	-1.113928079
H	0.043214001	-2.816600201	-1.333477094
H	-1.210508086	-3.335631239	-0.631496046
O	4.941989355	3.638169265	2.777887203
H	5.174479374	3.670417263	3.695798265
H	5.508603397	2.986799215	2.375154169
O	6.093939439	1.461641104	1.224228086
H	5.245637378	1.328072094	0.814657061
H	6.743421484	1.421733101	0.534089040
O	2.017982143	-2.575585185	-1.630225117
H	2.365878168	-2.620538189	-2.509862180
H	1.933163137	-1.650999118	-1.405254104

Coord_6

C	2.257724160	2.170684155	0.941449068
N	0.963111071	1.998059143	0.612281043
C	0.749486052	0.770583057	-0.063894004
C	2.839175204	0.953599067	-0.941952066
N	3.226491230	1.498967108	0.329537025
N	1.684699120	0.189250014	-0.753818055
H	3.632579264	0.516342039	-1.528692111
N	-0.446468030	0.229531018	0.119431008
H	-0.656644047	-0.641992044	-0.337430026
H	-1.209056087	0.804447057	0.435227030
H	2.534562185	2.870605206	1.714548125
O	-1.001793070	3.880736278	1.987489145
H	-0.314688020	3.419858249	1.517350112
H	-0.845672060	4.809354348	1.878264135
O	-2.819226201	2.031710144	0.761111055
H	-3.652968262	1.816355133	1.158111082
H	-2.463276178	2.779611199	1.235007088
O	-0.845481059	-2.574545188	-1.113748079
H	0.058392005	-2.800256202	-1.322373093
H	-1.203671084	-3.302405236	-0.622384043
O	4.966090357	3.625046261	2.753996199
H	5.192915375	3.659034263	3.673265263
H	5.523420397	2.960990214	2.359185171
O	6.086979440	1.417827101	1.219200087
H	5.232041375	1.262482092	0.832627058
H	6.719613482	1.373931097	0.513543035
O	2.031545146	-2.573416183	-1.591853114
H	2.404602174	-2.626772188	-2.460619179
H	1.959213141	-1.646841118	-1.369482097

Coord_7

C	2.226354162	2.199891156	0.934559069
N	0.946340068	2.015988145	0.617923047
C	0.749476056	0.795921059	-0.074250003
C	2.832369202	0.998036071	-0.953140069
N	3.199530232	1.487910108	0.356874025
N	1.703086124	0.203830017	-0.737709053
H	3.636408263	0.565223041	-1.529925109
N	-0.447766033	0.257981021	0.072241003
H	-0.648556049	-0.618028046	-0.380844029
H	-1.211681087	0.817192058	0.413193032
H	2.509626183	2.924790209	1.682869119
O	-1.019478073	3.864611279	1.998930143
H	-0.332890024	3.396055242	1.534788111
H	-0.867838062	4.791067342	1.867716135
O	-2.822382204	2.011927143	0.767382054
H	-3.651711265	1.788729128	1.169237082

H	-2.468490177	2.760691196	1.242041092
O	-0.826715058	-2.552287183	-1.109077079
H	0.078315005	-2.783734198	-1.307309094
H	-1.190951087	-3.271467238	-0.609426042
O	4.991531358	3.600594261	2.734630196
H	5.219930376	3.635555261	3.653478262
H	5.538734400	2.926878211	2.342113167
O	6.076980435	1.370368099	1.205772087
H	5.213674374	1.191941088	0.849635063
H	6.686497480	1.327330097	0.479934036
O	2.048911146	-2.567234186	-1.550073110
H	2.446801175	-2.627717188	-2.407247171
H	1.987588144	-1.639269116	-1.328939098

Coord_8

C	2.195213161	2.230110162	0.927406069
N	0.929356066	2.037313147	0.624003044
C	0.750047054	0.824221061	-0.082968008
C	2.823618203	1.046923073	-0.962053071
N	3.169563226	1.476650105	0.384319025
N	1.722706122	0.222162018	-0.718253053
H	3.638239264	0.619106043	-1.528936109
N	-0.447408034	0.289425019	0.026069002
H	-0.637483046	-0.591310040	-0.423057033
H	-1.213328088	0.831477060	0.390505028
H	2.485750177	2.979106216	1.649860117
O	-1.042685073	3.851187275	2.007470143
H	-0.355329023	3.375582242	1.550809111
H	-0.896324065	4.774982344	1.853807135
O	-2.826159201	1.991261142	0.769267057
H	-3.651228264	1.759178124	1.174805085
H	-2.476272178	2.741756197	1.244751088
O	-0.802896060	-2.531828180	-1.098957078
H	0.103508007	-2.767133199	-1.287397091
H	-1.171735084	-3.243215232	-0.591584043
O	5.018317363	3.563054258	2.721627194
H	5.257354378	3.597481260	3.637790262
H	5.554452399	2.883413205	2.324166168
O	6.063016437	1.319498094	1.182045087
H	5.190046371	1.116246082	0.865315061
H	6.641112477	1.283802093	0.430751032
O	2.070626151	-2.556771182	-1.504166110
H	2.493012182	-2.622938188	-2.349079172
H	2.018605143	-1.627964117	-1.282939090

Coord_9

C	2.164366154	2.261763163	0.919771068
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N	0.912083064	2.062549149	0.630496044
C	0.751202052	0.855925060	-0.089962006
C	2.812619201	1.100571079	-0.968472070
N	3.136348225	1.465376106	0.411625032
N	1.743640126	0.244737016	-0.695016049
H	3.637800264	0.678304049	-1.525446111
N	-0.445259030	0.324087023	-0.019360003
H	-0.623013044	-0.561655042	-0.464262033
H	-1.214072090	0.847464061	0.366658026
H	2.463422178	3.034008218	1.615000116
O	-1.072498078	3.840644275	2.012568146
H	-0.382871027	3.358732244	1.565136114
H	-0.932161065	4.761227344	1.836047131
O	-2.830879203	1.969711139	0.765739054
H	-3.651925264	1.727620126	1.173545082
H	-2.487225179	2.722841196	1.242199088
O	-0.773408054	-2.513958182	-1.082208078
H	0.134720008	-2.750831201	-1.261548089
H	-1.145057084	-3.218665233	-0.567630041
O	5.048277363	3.510364254	2.717710198
H	5.309581384	3.541720255	3.627889261
H	5.571546401	2.829344202	2.305810168
O	6.043544434	1.265596089	1.145612085
H	5.160397369	1.035387073	0.879440062
H	6.578711472	1.245523089	0.363117026
O	2.097394153	-2.541556183	-1.453217105
H	2.543899184	-2.611629188	-2.285285166
H	2.052512149	-1.612425118	-1.230580086

Coord_10

C	1.960190140	2.363459172	0.892644066
N	0.726979053	2.146382155	0.601789041
C	0.609903043	0.947599070	-0.138174011
C	2.663444193	1.245138091	-0.987650073
N	2.942320211	1.536921113	0.428147030
N	1.637797119	0.343685023	-0.700442052
H	3.511239254	0.842117058	-1.525882111
N	-0.577700040	0.403224031	-0.125317010
H	-0.724321054	-0.487630035	-0.571954043
H	-1.361940099	0.894596063	0.272525019
H	2.251025162	3.158563229	1.566614111
O	-1.316945094	3.855160279	1.960353142
H	-0.611701044	3.378714241	1.530852112
H	-1.192297086	4.774508344	1.766735125
O	-3.003507214	1.954026140	0.671291048
H	-3.822762275	1.688469122	1.067894077
H	-2.684354192	2.712490198	1.156845084

O	-0.824876061	-2.459091179	-1.135401081
H	0.090604009	-2.681868192	-1.295942091
H	-1.194415086	-3.165901229	-0.622222045
O	4.875634349	3.535517255	2.750792200
H	5.162452371	3.558971259	3.653501265
H	5.395831386	2.867035207	2.315225168
O	5.853267419	1.324488098	1.119094082
H	4.966794359	1.055052077	0.904882068
H	6.339486456	1.340098096	0.306075020
O	2.046741148	-2.441023174	-1.437621103
H	2.528015183	-2.502535182	-2.250758161
H	1.991091144	-1.513821108	-1.208409089

LIIC path connecting T₁/S₀ and S₀-MIN

Coord_1

C	1.960190140	2.363459172	0.892644066
N	0.726979053	2.146382155	0.601789041
C	0.609903043	0.947599070	-0.138174011
C	2.663444193	1.245138091	-0.987650073
N	2.942320211	1.536921113	0.428147030
N	1.637797119	0.343685023	-0.700442052
H	3.511239254	0.842117058	-1.525882111
N	-0.577700040	0.403224031	-0.125317010
H	-0.724321054	-0.487630035	-0.571954043
H	-1.361940099	0.894596063	0.272525019
H	2.251025162	3.158563229	1.566614111
O	-1.316945094	3.855160279	1.960353142
H	-0.611701044	3.378714241	1.530852112
H	-1.192297086	4.774508344	1.766735125
O	-3.003507214	1.954026140	0.671291048
H	-3.822762275	1.688469122	1.067894077
H	-2.684354192	2.712490198	1.156845084
O	-0.824876061	-2.459091179	-1.135401081
H	0.090604009	-2.681868192	-1.295942091
H	-1.194415086	-3.165901229	-0.622222045
O	4.875634349	3.535517255	2.750792200
H	5.162452371	3.558971259	3.653501265
H	5.395831386	2.867035207	2.315225168
O	5.853267419	1.324488098	1.119094082
H	4.966794359	1.055052077	0.904882068
H	6.339486456	1.340098096	0.306075020
O	2.046741148	-2.441023174	-1.437621103
H	2.528015183	-2.502535182	-2.250758161
H	1.991091144	-1.513821108	-1.208409089

Coord_2

C	1.978383143	2.341693170	0.875405064
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N	0.743468052	2.105040151	0.592155041
C	0.608816044	0.920363069	-0.151480009
C	2.706015195	1.131879083	-0.955241067
N	2.980773215	1.549269110	0.415263030
N	1.623791115	0.294893023	-0.718260054
H	3.550982254	0.705517053	-1.479229109
N	-0.594892041	0.403514030	-0.164062013
H	-0.746990055	-0.488625036	-0.604927046
H	-1.366932098	0.898992066	0.250780019
H	2.253891160	3.146410229	1.543861109
O	-1.236036089	3.838726278	1.985843145
H	-0.547650038	3.348571242	1.544768113
H	-1.095626082	4.755589342	1.791212128
O	-2.987375214	1.979476142	0.715646050
H	-3.799667271	1.720738123	1.130543080
H	-2.643594188	2.726009195	1.202553086
O	-0.865460061	-2.453493177	-1.141119084
H	0.041120004	-2.698183192	-1.317121093
H	-1.245518088	-3.154814225	-0.627898043
O	4.790070346	3.612950259	2.741939197
H	5.010451360	3.631353260	3.663199264
H	5.338288382	2.944484213	2.342278170
O	5.877038421	1.404955103	1.175080082
H	5.011260361	1.163358081	0.881449062
H	6.425537461	1.418516100	0.396617030
O	2.012137147	-2.480247178	-1.506825110
H	2.460146179	-2.538387184	-2.339539170
H	1.955580138	-1.554193109	-1.277401091

Coord_3

C	1.992258144	2.325895165	0.858727064
N	0.755418055	2.071772148	0.583132040
C	0.605362046	0.899861065	-0.162087013
C	2.740051199	1.027973072	-0.912249067
N	3.010305216	1.562469113	0.402452030
N	1.610370116	0.254618020	-0.729425053
H	3.582590260	0.578701043	-1.420222104
N	-0.612261046	0.408615029	-0.202026015
H	-0.767702058	-0.485944034	-0.635402046
H	-1.374806097	0.906026064	0.226504018
H	2.253687162	3.140351229	1.520519111
O	-1.174656084	3.826586274	2.002444144
H	-0.500077035	3.325183237	1.552949114
H	-1.021998074	4.740947341	1.805258128
O	-2.978056212	2.000415146	0.750578057
H	-3.783104272	1.745449123	1.181511083
H	-2.614440189	2.736933196	1.238006089

O	-0.894245065	-2.453067179	-1.143490084
H	0.004714001	-2.714813196	-1.331472094
H	-1.283001094	-3.150263227	-0.630978045
O	4.738664343	3.671165265	2.746845199
H	4.912237354	3.677316263	3.678180266
H	5.302276383	3.003787218	2.367380169
O	5.890697422	1.473845106	1.210132085
H	5.041028365	1.265668089	0.858917060
H	6.482551467	1.492303105	0.460715032
O	1.988830144	-2.509899180	-1.563939115
H	2.405681171	-2.562129187	-2.413538173
H	1.925634141	-1.585411112	-1.333931096

Coord_4

C	2.004165145	2.314111166	0.843049061
N	0.764882056	2.045293145	0.575334041
C	0.600569044	0.885184064	-0.170046013
C	2.766412200	0.932230070	-0.859735062
N	3.033539219	1.574356112	0.389750030
N	1.597932117	0.221336015	-0.734739051
H	3.606313260	0.460260035	-1.350654098
N	-0.629073044	0.418186031	-0.239075015
H	-0.786575058	-0.479628034	-0.663504046
H	-1.384423099	0.915870068	0.200458015
H	2.253277161	3.138088223	1.497302110
O	-1.128951082	3.818910273	2.012936147
H	-0.465468034	3.308247237	1.557575113
H	-0.966941070	4.730883342	1.812168130
O	-2.974093215	2.018376147	0.778112054
H	-3.771814270	1.764668127	1.223080089
H	-2.594588189	2.746539197	1.265658092
O	-0.913532068	-2.457190179	-1.143791080
H	-0.020830004	-2.731968196	-1.340772099
H	-1.309620096	-3.151609226	-0.632948045
O	4.708078337	3.712998267	2.760331197
H	4.851041350	3.703795266	3.696791266
H	5.280303383	3.048366221	2.389126173
O	5.899079426	1.532505108	1.227674088
H	5.059766362	1.359574100	0.836685059
H	6.519932469	1.561941111	0.501447038
O	1.975251144	-2.531684180	-1.611261118
H	2.362744169	-2.575966187	-2.475503178
H	1.900634135	-1.609315117	-1.379959098

Coord_5

C	2.015485146	2.305044168	0.828658059
N	0.773008055	2.024702144	0.569119040

C	0.594928041	0.875735064	-0.175460015
C	2.785426200	0.844011063	-0.798698059
N	3.052281222	1.583634113	0.377250027
N	1.586496115	0.194075015	-0.734818052
H	3.622002259	0.349407027	-1.272119093
N	-0.644991045	0.431980030	-0.275143022
H	-0.803865057	-0.469712035	-0.689311047
H	-1.395153099	0.928598067	0.173147013
H	2.254362165	3.138115227	1.474727107
O	-1.096449079	3.815684276	2.019221148
H	-0.441595033	3.297455238	1.560113110
H	-0.927557064	4.725464339	1.814199133
O	-2.974640214	2.034308145	0.799665057
H	-3.765064270	1.779694130	1.256867093
H	-2.582611188	2.755584197	1.287218091
O	-0.924858064	-2.465726178	-1.142959081
H	-0.036972000	-2.749934198	-1.346330095
H	-1.327105096	-3.158788230	-0.634923046
O	4.690888337	3.740524268	2.778249202
H	4.816275346	3.715041267	3.716883269
H	5.268087379	3.080544219	2.406543175
O	5.905024425	1.582050116	1.230927089
H	5.070222364	1.444116103	0.814559057
H	6.544081473	1.627498118	0.522689039
O	1.970305141	-2.546565184	-1.650450118
H	2.329989166	-2.581126184	-2.527422181
H	1.880007134	-1.627059118	-1.416912101

Coord_6

C	2.026902145	2.297722165	0.815825061
N	0.780305054	2.009308145	0.564708040
C	0.588535040	0.871080061	-0.178441013
C	2.797092204	0.762947056	-0.729931053
N	3.067695219	1.589468112	0.365213028
N	1.575814112	0.172155012	-0.730068051
H	3.629267260	0.245622018	-1.185896084
N	-0.659989050	0.449794031	-0.310259024
H	-0.819977060	-0.456234034	-0.712934049
H	-1.406771101	0.944228068	0.144818012
H	2.257821163	3.139321227	1.453268107
O	-1.075695076	3.816803274	2.022554144
H	-0.427171032	3.292509236	1.561533110
H	-0.902066067	4.724631340	1.812872131
O	-2.979337213	2.048824149	0.816077061
H	-3.762587271	1.791395128	1.283828092
H	-2.577758188	2.764525197	1.303749096
O	-0.929291067	-2.479036177	-1.141843084

H	-0.044683002	-2.769186200	-1.349265097
H	-1.336553096	-3.172352228	-0.638005048
O	4.683880337	3.755735272	2.797948201
H	4.802543345	3.714282268	3.736848269
H	5.263810378	3.102249223	2.419187172
O	5.910157424	1.623420119	1.222451088
H	5.074311365	1.519136111	0.792807057
H	6.558887471	1.688697123	0.527620039
O	1.973208144	-2.555069184	-1.682706122
H	2.306472164	-2.578181186	-2.570724184
H	1.863186135	-1.639442120	-1.445742106

Coord_7

C	2.038550146	2.291238167	0.805003058
N	0.786776056	1.998478146	0.562328039
C	0.581168041	0.870828062	-0.179029014
C	2.801181204	0.688709050	-0.653779049
N	3.080424223	1.591141117	0.354286026
N	1.565439110	0.155000012	-0.720569050
H	3.627528261	0.148365013	-1.092690079
N	-0.674308047	0.471435036	-0.344545026
H	-0.835477058	-0.439256032	-0.734549055
H	-1.419405102	0.962750071	0.115444007
H	2.263901161	3.140678228	1.433584105
O	-1.066086079	3.822105275	2.023679143
H	-0.421680029	3.293094236	1.562454111
H	-0.889555063	4.728242340	1.809143130
O	-2.988272217	2.062378151	0.827541061
H	-3.764599272	1.800439127	1.304149096
H	-2.579870187	2.773684202	1.315657093
O	-0.927646066	-2.497971181	-1.141419080
H	-0.044668005	-2.790434202	-1.350790096
H	-1.338732094	-3.193570230	-0.643720046
O	4.687093337	3.760837271	2.818296204
H	4.809230346	3.704713267	3.755948271
H	5.267773381	3.115487222	2.427036172
O	5.915436427	1.657609118	1.204041085
H	5.073188366	1.584795112	0.772449058
H	6.566108470	1.745203125	0.517787037
O	1.983332141	-2.557452186	-1.708949123
H	2.291584164	-2.567024187	-2.606447189
H	1.849594132	-1.647144120	-1.466849108

Coord_8

C	2.049901146	2.284367165	0.797349060
N	0.791831059	1.991358145	0.562501038
C	0.572259040	0.874343063	-0.176920015

C	2.797246200	0.620592047	-0.569386041
N	3.090541224	1.587581114	0.346251025
N	1.554752111	0.141759012	-0.705577051
H	3.616006263	0.056558004	-0.991735072
N	-0.688433052	0.496489034	-0.378204028
H	-0.851066059	-0.419088029	-0.754390054
H	-1.433585105	0.983968073	0.084572007
H	2.272061164	3.140874225	1.417033102
O	-1.068153077	3.831314277	2.022692143
H	-0.425598031	3.298752236	1.563155112
H	-0.890155065	4.736001343	1.803283132
O	-3.002159215	2.075265152	0.833110059
H	-3.772109270	1.807376128	1.316609093
H	-2.589614187	2.783235200	1.322269094
O	-0.920889066	-2.523695181	-1.143106082
H	-0.037885000	-2.814530203	-1.352941096
H	-1.334707098	-3.224681233	-0.655187047
O	4.704659339	3.758934270	2.840015205
H	4.842849347	3.691057266	3.774617274
H	5.283285381	3.123266223	2.430387177
O	5.921585424	1.686222124	1.176600086
H	5.067119364	1.641031117	0.756373055
H	6.564784474	1.797027130	0.491468036
O	1.999750145	-2.553867185	-1.730279125
H	2.284991166	-2.545976183	-2.635613189
H	1.838740130	-1.651178117	-1.479454104

Coord_9

C	2.059229149	2.274073165	0.796848056
N	0.793954060	1.985232141	0.567164042
C	0.561281041	0.878621065	-0.169842010
C	2.785146202	0.555280039	-0.470728034
N	3.097486220	1.575589111	0.347599024
N	1.543816113	0.128880008	-0.680444047
H	3.594531261	-0.033937005	-0.875709060
N	-0.702407052	0.521983037	-0.410860032
H	-0.866565063	-0.398865028	-0.771618054
H	-1.450010105	1.005466074	0.050954001
H	2.279876165	3.137219224	1.407421100
O	-1.085312078	3.843389276	2.017105143
H	-0.441700032	3.307942240	1.562609113
H	-0.906601063	4.746664344	1.792500130
O	-3.022947218	2.086103151	0.828100058
H	-3.787994272	1.811422132	1.315461096
H	-2.609567186	2.792048203	1.319158098
O	-0.912878068	-2.553692186	-1.148267084
H	-0.029698004	-2.839755204	-1.362235099

H	-1.330434097	-3.267708238	-0.682821048
O	4.750859344	3.757599273	2.867528204
H	4.929543355	3.686387266	3.794950275
H	5.321666385	3.133903225	2.429594173
O	5.929975429	1.714215124	1.139860082
H	5.054982361	1.686213123	0.754632052
H	6.546727470	1.846120131	0.437748031
O	2.017567146	-2.545496183	-1.751902128
H	2.285590163	-2.504650181	-2.662280193
H	1.831894132	-1.655891118	-1.477034108

Coord_10

C	2.010404145	2.225413158	0.765495055
N	0.733465052	1.970661140	0.527942038
C	0.473481037	0.886914066	-0.219420018
C	2.683538196	0.459482034	-0.411087028
N	3.035677217	1.507145108	0.318932022
N	1.446775102	0.107636007	-0.709087052
H	3.471976249	-0.166874013	-0.800625058
N	-0.794624056	0.576531040	-0.514996040
H	-0.974985073	-0.343057027	-0.869526064
H	-1.541119113	1.064285077	-0.057112005
H	2.243360162	3.084142222	1.377352101
O	-1.151952084	3.867401276	1.967531141
H	-0.511431036	3.323101237	1.519413109
H	-0.955890071	4.768363342	1.748159125
O	-3.108885222	2.151434157	0.743146053
H	-3.878275281	1.877573136	1.223994089
H	-2.688481193	2.843955204	1.246873089
O	-0.991563074	-2.610662186	-1.235090089
H	-0.096889005	-2.891674207	-1.401037101
H	-1.415368104	-3.306666240	-0.748383056
O	4.834936348	3.676631264	2.879494209
H	5.122060367	3.616109262	3.780013273
H	5.373438388	3.071854219	2.378706171
O	5.880408423	1.667978119	1.026812073
H	4.971025359	1.635707118	0.740742054
H	6.411359463	1.811739131	0.255726017
O	1.965991140	-2.557345186	-1.762375127
H	2.207905159	-2.559217182	-2.678387195
H	1.716794122	-1.666433123	-1.540605113

LIIC path connecting Franck-Condon point and S_2/S_1

Coord_1

C	2.010404145	2.225413158	0.765495055
N	0.733465052	1.970661140	0.527942038
C	0.473481037	0.886914066	-0.219420018

C	2.683538196	0.459482034	-0.411087028
N	3.035677217	1.507145108	0.318932022
N	1.446775102	0.107636007	-0.709087052
H	3.471976249	-0.166874013	-0.800625058
N	-0.794624056	0.576531040	-0.514996040
H	-0.974985073	-0.343057027	-0.869526064
H	-1.541119113	1.064285077	-0.057112005
H	2.243360162	3.084142222	1.377352101
O	-1.151952084	3.867401276	1.967531141
H	-0.511431036	3.323101237	1.519413109
H	-0.955890071	4.768363342	1.748159125
O	-3.108885222	2.151434157	0.743146053
H	-3.878275281	1.877573136	1.223994089
H	-2.688481193	2.843955204	1.246873089
O	-0.991563074	-2.610662186	-1.235090089
H	-0.096889005	-2.891674207	-1.401037101
H	-1.415368104	-3.306666240	-0.748383056
O	4.834936348	3.676631264	2.879494209
H	5.122060367	3.616109262	3.780013273
H	5.373438388	3.071854219	2.378706171
O	5.880408423	1.667978119	1.026812073
H	4.971025359	1.635707118	0.740742054
H	6.411359463	1.811739131	0.255726017
O	1.965991140	-2.557345186	-1.762375127
H	2.207905159	-2.559217182	-2.678387195
H	1.716794122	-1.666433123	-1.540605113

Coord_2

C	2.015985144	2.231212163	0.765101056
N	0.734715053	1.961722140	0.526398037
C	0.474444033	0.875387061	-0.217890018
C	2.689610193	0.460494032	-0.417237031
N	3.038597217	1.510614109	0.313558020
N	1.448453102	0.099758008	-0.711395053
H	3.480176253	-0.160799011	-0.809503060
N	-0.793772060	0.559912038	-0.502044035
H	-0.975039070	-0.356103024	-0.866107060
H	-1.541263113	1.053772077	-0.051720006
H	2.244806160	3.088211225	1.379540100
O	-1.160500085	3.875311280	1.972779140
H	-0.510663036	3.333843239	1.535759109
H	-0.961094069	4.777464344	1.761145129
O	-3.101496225	2.148738153	0.735065051
H	-3.875979277	1.877636134	1.209351088
H	-2.687304192	2.845219202	1.238443089
O	-1.001176071	-2.606210186	-1.242875091
H	-0.106180008	-2.884800205	-1.411924102

H	-1.418198102	-3.299771235	-0.747026055
O	4.834810346	3.680526263	2.881109210
H	5.121408367	3.615785263	3.781520270
H	5.372513386	3.076664223	2.378351172
O	5.883110423	1.673393121	1.027894077
H	4.974847357	1.639168117	0.738737054
H	6.416755463	1.813057131	0.257908021
O	1.954892139	-2.564702184	-1.762001126
H	2.205529159	-2.562617183	-2.675587191
H	1.715700122	-1.671942122	-1.535221110

Coord_3

C	2.021528144	2.237091163	0.764738057
N	0.736052051	1.952893140	0.524950038
C	0.475416037	0.863983064	-0.216239017
C	2.695509196	0.461531034	-0.423347033
N	3.041405217	1.514083109	0.308217024
N	1.450008105	0.091915008	-0.713591049
H	3.488122252	-0.154735010	-0.818349057
N	-0.792778058	0.543427040	-0.489026036
H	-0.974858070	-0.368966027	-0.862502061
H	-1.541235109	1.043278074	-0.046319001
H	2.246395163	3.092309221	1.381723099
O	-1.168937086	3.883246277	1.977736144
H	-0.509983038	3.344634242	1.551989113
H	-0.966414068	4.786561345	1.773832127
O	-3.093829225	2.145921157	0.727079052
H	-3.873334279	1.877578136	1.194755088
H	-2.685828194	2.846373206	1.229970088
O	-1.010805075	-2.601904186	-1.250744089
H	-0.115418008	-2.877931210	-1.422724102
H	-1.421040101	-3.293013235	-0.746019052
O	4.834645348	3.684451265	2.882668208
H	5.120724369	3.615545260	3.782954271
H	5.371510389	3.081447223	2.377981171
O	5.885689421	1.678721121	1.029021076
H	4.978556360	1.642523116	0.736786052
H	6.422019464	1.814222131	0.260150018
O	1.943641137	-2.571797186	-1.761684128
H	2.202975159	-2.565677182	-2.672750193
H	1.714332125	-1.677450122	-1.529632109

Coord_4

C	2.027034148	2.243053160	0.764409057
N	0.737474051	1.944177141	0.523602039
C	0.476394036	0.852703064	-0.214463013
C	2.701235195	0.462596035	-0.429416029

N	3.044102222	1.517554110	0.302910022
N	1.451438106	0.084109004	-0.715670054
H	3.495812250	-0.148681011	-0.827163059
N	-0.791648059	0.527080040	-0.475940033
H	-0.974445068	-0.381644029	-0.858721063
H	-1.541044113	1.032805074	-0.040912005
H	2.248128160	3.096440222	1.383904098
O	-1.177265087	3.891190281	1.982427142
H	-0.509396037	3.355456240	1.568125113
H	-0.971842072	4.795635343	1.786251129
O	-3.085895223	2.142991156	0.719182050
H	-3.870357276	1.877405138	1.180191082
H	-2.684064193	2.847417204	1.221458086
O	-1.020444076	-2.597769190	-1.258685092
H	-0.124593011	-2.871078205	-1.433427103
H	-1.423887101	-3.286428237	-0.745351055
O	4.834452347	3.688407268	2.884169209
H	5.120021367	3.615388258	3.784311272
H	5.370438387	3.086202225	2.377589173
O	5.888148423	1.683958124	1.030184075
H	4.982155358	1.645771116	0.734885051
H	6.427149462	1.815229129	0.262441017
O	1.932249137	-2.578623186	-1.761423127
H	2.200251161	-2.568380183	-2.669879194
H	1.712691125	-1.682955121	-1.523836110

Coord_5

C	2.032501147	2.249099163	0.764116056
N	0.738976052	1.935575137	0.522357038
C	0.477376035	0.841550060	-0.212560018
C	2.706785196	0.463690035	-0.435442030
N	3.046685220	1.521030111	0.297636019
N	1.452740104	0.076342005	-0.717630052
H	3.503247254	-0.142636013	-0.835947058
N	-0.790385055	0.510869039	-0.462784031
H	-0.973802070	-0.394134030	-0.854775063
H	-1.540695110	1.022351072	-0.035497003
H	2.250003162	3.100609223	1.386085102
O	-1.185492084	3.899121282	1.986876141
H	-0.508912036	3.366289244	1.584190114
H	-0.977375070	4.804667346	1.798429127
O	-3.077702220	2.139953154	0.711368049
H	-3.867063280	1.877126134	1.165641084
H	-2.682018192	2.848348206	1.212911085
O	-1.030088072	-2.593827184	-1.266685093
H	-0.133697008	-2.864253205	-1.444023105
H	-1.426732101	-3.280052234	-0.745011054

O	4.834243348	3.692391268	2.885606206
H	5.119313371	3.615312263	3.785586272
H	5.369304387	3.090926222	2.377170170
O	5.890488424	1.689103124	1.031374073
H	4.985644356	1.648908116	0.733028052
H	6.432146461	1.816075130	0.264773022
O	1.920730139	-2.585174184	-1.761216129
H	2.197363160	-2.570707187	-2.666972191
H	1.710776123	-1.688453119	-1.517829107

Coord_6

C	2.037933147	2.255229163	0.763861056
N	0.740557053	1.927091140	0.521217037
C	0.478359035	0.830526060	-0.210526014
C	2.712157197	0.464814034	-0.441425029
N	3.049155219	1.524512108	0.292397021
N	1.453913105	0.068614006	-0.719469054
H	3.510425252	-0.136599010	-0.844699062
N	-0.788993055	0.494798037	-0.449555033
H	-0.972932071	-0.406432030	-0.850672060
H	-1.540196112	1.011918073	-0.030074000
H	2.252020164	3.104821226	1.388265101
O	-1.193623088	3.907021280	1.991109141
H	-0.508538035	3.377113242	1.600207114
H	-0.983011072	4.813641345	1.810396132
O	-3.069259223	2.136811154	0.703630049
H	-3.863466277	1.876745137	1.151090080
H	-2.679699195	2.849164203	1.204333085
O	-1.039727073	-2.590103184	-1.274732091
H	-0.142721009	-2.857468206	-1.454503106
H	-1.429567105	-3.273923234	-0.744988056
O	4.834028349	3.696402268	2.886975209
H	5.118611369	3.615316258	3.786776275
H	5.368119384	3.095616224	2.376717173
O	5.892711423	1.694150120	1.032583074
H	4.989022359	1.651932121	0.731210053
H	6.437007462	1.816753133	0.267134020
O	1.909098140	-2.591442188	-1.761061127
H	2.194320158	-2.572641187	-2.664027193
H	1.708589123	-1.693940121	-1.511607110

Coord_7

C	2.043328146	2.261446165	0.763645057
N	0.742215056	1.918725139	0.520185035
C	0.479341034	0.819632057	-0.208357017
C	2.717351193	0.465969032	-0.447364033
N	3.051509221	1.528002111	0.287192023

N	1.454954103	0.060927002	-0.721182054
H	3.517344255	-0.130569009	-0.853421062
N	-0.787474057	0.478867034	-0.436250030
H	-0.971836071	-0.418534028	-0.846423063
H	-1.539552108	1.001506071	-0.024643001
H	2.254180165	3.109080224	1.390447100
O	-1.201667085	3.914871280	1.995148145
H	-0.508284035	3.387910241	1.616200115
H	-0.988748073	4.822537349	1.822180131
O	-3.060574218	2.133568155	0.695965049
H	-3.859580280	1.876265137	1.136521079
H	-2.677113190	2.849860203	1.195730087
O	-1.049356077	-2.586626188	-1.282815093
H	-0.151654013	-2.850739204	-1.464855104
H	-1.432384106	-3.268080233	-0.745273055
O	4.833819350	3.700438266	2.888271206
H	5.117931366	3.615398259	3.787875270
H	5.366889386	3.100269222	2.376223171
O	5.894819422	1.699096123	1.033802076
H	4.992292357	1.654839119	0.729428054
H	6.441732465	1.817259132	0.269515021
O	1.897365137	-2.597419187	-1.760957128
H	2.191133156	-2.574161185	-2.661045194
H	1.706127121	-1.699414121	-1.505165107

Coord_8

C	2.048690145	2.267750164	0.763469053
N	0.743948053	1.910481139	0.519264039
C	0.480320033	0.808871058	-0.206051016
C	2.722365195	0.467155035	-0.453259031
N	3.053749218	1.531501110	0.282021020
N	1.455862107	0.053283005	-0.722768051
H	3.524004253	-0.124546009	-0.862113063
N	-0.785833057	0.463077031	-0.422868032
H	-0.970515070	-0.430435029	-0.842036062
H	-1.538769111	0.991114072	-0.019205001
H	2.256483160	3.113389224	1.392630099
O	-1.209631086	3.922654282	1.999020145
H	-0.508161038	3.398661244	1.632194116
H	-0.994589073	4.831338350	1.833811130
O	-3.051653221	2.130227152	0.688366048
H	-3.855415279	1.875692133	1.121920079
H	-2.674269191	2.850434207	1.187105085
O	-1.058967079	-2.583422184	-1.290924094
H	-0.160488014	-2.844080207	-1.475071104
H	-1.435175103	-3.262561232	-0.745856055
O	4.833627349	3.704498267	2.889487208

H	5.117286368	3.615555261	3.788877273
H	5.365625388	3.104882224	2.375682171
O	5.896815426	1.703936121	1.035024073
H	4.995453360	1.657625121	0.727674053
H	6.446320463	1.817586132	0.271906019
O	1.885546138	-2.603100190	-1.760900125
H	2.187809156	-2.575250184	-2.658021190
H	1.703393121	-1.704871124	-1.498501109

Coord_9

C	2.054021146	2.274143165	0.763334054
N	0.745756056	1.902360137	0.518455038
C	0.481297032	0.798244057	-0.203604016
C	2.727198198	0.468373032	-0.459108032
N	3.055874219	1.535011111	0.276884021
N	1.456636103	0.045683004	-0.724222050
H	3.530404255	-0.118530010	-0.870774065
N	-0.784071055	0.447428032	-0.409406027
H	-0.968969068	-0.442131031	-0.837520058
H	-1.537850110	0.980743071	-0.013759000
H	2.258930160	3.117753222	1.394814098
O	-1.217526088	3.930353281	2.002748146
H	-0.508181036	3.409349244	1.648213121
H	-1.000537073	4.840028351	1.845319131
O	-3.042504217	2.126789151	0.680829050
H	-3.850983277	1.875025137	1.107269082
H	-2.671174192	2.850882203	1.178464086
O	-1.068552077	-2.580521186	-1.299050092
H	-0.169212014	-2.837508206	-1.485139109
H	-1.437933106	-3.257410237	-0.746729054
O	4.833465346	3.708579266	2.890620208
H	5.116689366	3.615787258	3.789777271
H	5.364337386	3.109452225	2.375086170
O	5.898702424	1.708667124	1.036238075
H	4.998508359	1.660287120	0.725945051
H	6.450771463	1.817727131	0.274298022
O	1.873656134	-2.608477187	-1.760887129
H	2.184361159	-2.575886186	-2.654953189
H	1.700386124	-1.710309124	-1.491610105

Coord_10

C	2.060445146	2.282308163	0.775020055
N	0.748986053	1.894929139	0.530101039
C	0.484232034	0.790414060	-0.192116012
C	2.733902196	0.476579036	-0.460365035
N	3.059404218	1.543423109	0.279551021
N	1.459598104	0.044074004	-0.720645050

H	3.538865254	-0.102917006	-0.878035064
N	-0.779972054	0.433360029	-0.386366026
H	-0.964289067	-0.450938033	-0.826183060
H	-1.534823111	0.969351071	0.004144003
H	2.262306163	3.121963224	1.411395100
O	-1.224910090	3.930384281	2.028615145
H	-0.507626035	3.414655246	1.683714120
H	-1.007725073	4.841864347	1.881828134
O	-3.031892219	2.117598151	0.691950049
H	-3.844069275	1.865938137	1.111465082
H	-2.666964190	2.844367206	1.190400086
O	-1.072698075	-2.573787184	-1.307675094
H	-0.172309013	-2.824868204	-1.497719107
H	-1.433421103	-3.250974235	-0.750194054
O	4.835406347	3.711157270	2.904373207
H	5.119665369	3.611883258	3.802531274
H	5.365238384	3.115043226	2.384304173
O	5.902844427	1.719795124	1.041696078
H	5.003443360	1.669064118	0.729622050
H	6.456185465	1.827653131	0.280503022
O	1.866502134	-2.603386189	-1.765776128
H	2.184240157	-2.562330184	-2.657024193
H	1.700955122	-1.706777125	-1.486005107

LIIC path connecting S₂/S₁ and S2-MIN

Coord_1

C	2.060445146	2.282308163	0.775020055
N	0.748986053	1.894929139	0.530101039
C	0.484232034	0.790414060	-0.192116012
C	2.733902196	0.476579036	-0.460365035
N	3.059404218	1.543423109	0.279551021
N	1.459598104	0.044074004	-0.720645050
H	3.538865254	-0.102917006	-0.878035064
N	-0.779972054	0.433360029	-0.386366026
H	-0.964289067	-0.450938033	-0.826183060
H	-1.534823111	0.969351071	0.004144003
H	2.262306163	3.121963224	1.411395100
O	-1.224910090	3.930384281	2.028615145
H	-0.507626035	3.414655246	1.683714120
H	-1.007725073	4.841864347	1.881828134
O	-3.031892219	2.117598151	0.691950049
H	-3.844069275	1.865938137	1.111465082
H	-2.666964190	2.844367206	1.190400086
O	-1.072698075	-2.573787184	-1.307675094
H	-0.172309013	-2.824868204	-1.497719107
H	-1.433421103	-3.250974235	-0.750194054
O	4.835406347	3.711157270	2.904373207

H	5.119665369	3.611883258	3.802531274
H	5.365238384	3.115043226	2.384304173
O	5.902844427	1.719795124	1.041696078
H	5.003443360	1.669064118	0.729622050
H	6.456185465	1.827653131	0.280503022
O	1.866502134	-2.603386189	-1.765776128
H	2.184240157	-2.562330184	-2.657024193
H	1.700955122	-1.706777125	-1.486005107

Coord_2

C	2.061352150	2.260819164	0.781674057
N	0.744373051	1.901330136	0.535851037
C	0.468883031	0.803449060	-0.187289016
C	2.730593198	0.487863037	-0.503307038
N	3.057499222	1.535198112	0.270861021
N	1.443389103	0.053686006	-0.712015053
H	3.530942253	-0.095236008	-0.924166065
N	-0.795110058	0.446491034	-0.383904029
H	-0.977328068	-0.437808034	-0.823391057
H	-1.549161110	0.977881069	0.013910001
H	2.272135165	3.090381222	1.429600104
O	-1.219082086	3.920962285	2.022125146
H	-0.507563036	3.401118246	1.669444120
H	-1.001121073	4.831017346	1.868317132
O	-3.048644219	2.124141153	0.701032048
H	-3.855080278	1.873964136	1.132180080
H	-2.672179195	2.846694205	1.197318084
O	-1.038621076	-2.572249183	-1.289547090
H	-0.134918010	-2.815619202	-1.472730108
H	-1.401065099	-3.255667233	-0.740905051
O	4.839820347	3.712291265	2.906954211
H	5.128036371	3.620205263	3.804624275
H	5.363014385	3.107692224	2.390031172
O	5.895444423	1.706761123	1.050321074
H	4.997089360	1.656778120	0.734244054
H	6.450620462	1.825479133	0.292072022
O	1.866424133	-2.603154187	-1.765604125
H	2.184260155	-2.562299185	-2.657086192
H	1.701015120	-1.707042121	-1.486117107

Coord_3

C	2.061702148	2.239459163	0.787193058
N	0.739618055	1.907931135	0.541119039
C	0.453585030	0.816264061	-0.182336012
C	2.725406197	0.500855037	-0.546328037
N	3.054991218	1.526932109	0.261816021
N	1.427959104	0.063736002	-0.702777052

H	3.519943251	-0.087114005	-0.970779071
N	-0.810191059	0.459466031	-0.381236028
H	-0.990722074	-0.424957028	-0.820045059
H	-1.563355115	0.986411073	0.023662002
H	2.281401164	3.058829219	1.446314104
O	-1.212450087	3.912375283	2.013533143
H	-0.507004034	3.388055246	1.653300118
H	-0.993685069	4.820830345	1.852072132
O	-3.064986223	2.131165155	0.709847051
H	-3.865487279	1.882899135	1.152825083
H	-2.676790191	2.849670208	1.203262089
O	-1.002368074	-2.569651187	-1.271660090
H	-0.095208004	-2.803967201	-1.448354103
H	-1.365140097	-3.260295237	-0.732412053
O	4.843532351	3.712444266	2.909638209
H	5.135363369	3.627222259	3.806814275
H	5.360020385	3.099365223	2.396005171
O	5.887148426	1.692589121	1.059363078
H	4.989937360	1.643731117	0.739016052
H	6.444406466	1.821967132	0.304378023
O	1.866345132	-2.602922185	-1.765432126
H	2.184280158	-2.562267185	-2.657147190
H	1.701074124	-1.707306122	-1.486228108

Coord_4

C	2.061534150	2.218274160	0.791514055
N	0.734763055	1.914765136	0.545830039
C	0.438377032	0.828852061	-0.177294011
C	2.718399197	0.515480036	-0.589299045
N	3.051922218	1.518570109	0.252414018
N	1.413378101	0.074240007	-0.692934049
H	3.505843255	-0.078759006	-1.017613073
N	-0.825181058	0.472264035	-0.378362029
H	-1.004441073	-0.412429032	-0.816107060
H	-1.577362114	0.994939071	0.033398001
H	2.290144167	3.027395217	1.461436106
O	-1.205081088	3.904734281	2.002647142
H	-0.506011039	3.375580242	1.635108116
H	-0.985550070	4.811401349	1.832830130
O	-3.080914220	2.138634154	0.718379050
H	-3.875248282	1.892709134	1.173430086
H	-2.680820193	2.853304205	1.208154089
O	-0.963923072	-2.565852187	-1.254187091
H	-0.053203004	-2.789761199	-1.424830100
H	-1.325559094	-3.264722233	-0.724916050
O	4.846554350	3.711668270	2.912357211
H	5.141627368	3.633035261	3.809061273

H	5.356254384	3.090068224	2.402211171
O	5.877953421	1.677187121	1.068909076
H	4.982000357	1.629842119	0.743995055
H	6.437582461	1.816956131	0.317527024
O	1.866266137	-2.602689189	-1.765260128
H	2.184300155	-2.562236186	-2.657208193
H	1.701133122	-1.707571124	-1.486339108

Coord_5

C	2.060898148	2.197314158	0.794573059
N	0.729867054	1.921865139	0.549898041
C	0.423313028	0.841207058	-0.172202013
C	2.709653194	0.531655037	-0.632093048
N	3.048351219	1.510057107	0.242653016
N	1.399729101	0.085215005	-0.682490048
H	3.488606253	-0.070413007	-1.064401078
N	-0.840025062	0.484862036	-0.375283027
H	-1.018436076	-0.400269031	-0.811532058
H	-1.591125115	1.003467075	0.043117002
H	2.298410164	2.996176215	1.474867106
O	-1.197065084	3.898150279	1.989271144
H	-0.504657038	3.363814240	1.614701115
H	-0.976882072	4.802823348	1.810332128
O	-3.096420225	2.146490155	0.726612053
H	-3.884312278	1.903339136	1.194012086
H	-2.684299195	2.857587207	1.211911089
O	-0.923285064	-2.560712182	-1.237307088
H	-0.008955002	-2.772860199	-1.402403103
H	-1.282258092	-3.268799237	-0.718630049
O	4.848898351	3.710018268	2.915044209
H	5.146807372	3.637750262	3.811321273
H	5.351714387	3.079808224	2.408638172
O	5.867859424	1.660471121	1.079058076
H	4.973300360	1.615030115	0.749244054
H	6.430194464	1.810289132	0.331632022
O	1.866187136	-2.602456187	-1.765088129
H	2.184319158	-2.562204187	-2.657269192
H	1.701192125	-1.707835125	-1.486450108

Coord_6

C	2.059861146	2.176636155	0.796304056
N	0.725006053	1.929269139	0.553233038
C	0.408467029	0.853322063	-0.167099014
C	2.699268196	0.549290038	-0.674593051
N	3.044350220	1.501335107	0.232525018
N	1.387116098	0.096677006	-0.671446050
H	3.468181249	-0.062356003	-1.110863079

N	-0.854654061	0.497232036	-0.371998027
H	-1.032637076	-0.388525027	-0.806270057
H	-1.604562116	1.011994073	0.052820002
H	2.306263165	2.965281212	1.486502105
O	-1.188510087	3.892727281	1.973214145
H	-0.503031035	3.352876241	1.591920113
H	-0.967880069	4.795189347	1.784326130
O	-3.111491224	2.154658154	0.734525052
H	-3.892624282	1.914708139	1.214578089
H	-2.687259196	2.862495204	1.214447086
O	-0.880477064	-2.554093186	-1.221205087
H	0.037455002	-2.753142197	-1.381322099
H	-1.235205090	-3.272357235	-0.713776049
O	4.850578351	3.707554266	2.917628208
H	5.150884371	3.641476262	3.813551273
H	5.346402384	3.068600223	2.415275176
O	5.856873423	1.642356119	1.089912078
H	4.963863357	1.599220114	0.754828054
H	6.422298462	1.801812131	0.346812027
O	1.866109135	-2.602223190	-1.764916125
H	2.184339155	-2.562173182	-2.657330190
H	1.701251123	-1.708100121	-1.486561108

Coord_7

C	2.058507151	2.156301154	0.796637057
N	0.720272054	1.937020141	0.555730040
C	0.393933028	0.865190065	-0.162029009
C	2.687368196	0.568293042	-0.716692054
N	3.040008221	1.492344105	0.222020014
N	1.375657098	0.108649006	-0.659803050
H	3.444487248	-0.054904002	-1.156716081
N	-0.868976063	0.509347035	-0.368505029
H	-1.046953078	-0.377252027	-0.800261059
H	-1.617573118	1.020520071	0.062505004
H	2.313779165	2.934829210	1.496232108
O	-1.179551085	3.888561281	1.954302138
H	-0.501234034	3.342886243	1.566626113
H	-0.958775072	4.788575346	1.754579124
O	-3.126112222	2.163038157	0.742091054
H	-3.900122279	1.926706137	1.235126089
H	-2.689745196	2.867987207	1.215680090
O	-0.835545058	-2.545863183	-1.206066088
H	0.085918007	-2.730509196	-1.361834100
H	-1.184400084	-3.275219237	-0.710580051
O	4.851612348	3.704339265	2.920039209
H	5.153837371	3.644329263	3.815702273
H	5.340323386	3.056462220	2.422113173

O	5.845006422	1.622769115	1.101583077
H	4.953731359	1.582338116	0.760818054
H	6.413956464	1.791374131	0.363197027
O	1.866030134	-2.601990188	-1.764744127
H	2.184359158	-2.562141183	-2.657391193
H	1.701310121	-1.708364122	-1.486672109

Coord_8

C	2.056938151	2.136378155	0.795496056
N	0.715779054	1.945166142	0.557274042
C	0.379825030	0.876806061	-0.157037011
C	2.674102193	0.588571040	-0.758295054
N	3.035433219	1.483025109	0.211121016
N	1.365495096	0.121159010	-0.647567048
H	3.417399247	-0.048410003	-1.201665085
N	-0.882877063	0.521173036	-0.364799026
H	-1.061269074	-0.366507025	-0.793440059
H	-1.630037116	1.029044074	0.072171003
H	2.321053167	2.904952212	1.503941110
O	-1.170343083	3.885732278	1.932379140
H	-0.499379035	3.333950238	1.538708113
H	-0.949832066	4.783044343	1.720893124
O	-3.140261226	2.171512158	0.749285054
H	-3.906740281	1.939201139	1.255638090
H	-2.691803193	2.874000206	1.215528089
O	-0.788556055	-2.535904183	-1.192070085
H	0.136294009	-2.704889196	-1.344183096
H	-1.129879079	-3.277195238	-0.709265051
O	4.852022349	3.700441266	2.922203210
H	5.155643373	3.646431261	3.817726275
H	5.333483384	3.043422218	2.429148177
O	5.832275418	1.601639115	1.114192080
H	4.942948357	1.564316111	0.767287056
H	6.405236459	1.778835128	0.380926025
O	1.865951133	-2.601757186	-1.764572129
H	2.184378156	-2.562110184	-2.657452192
H	1.701369124	-1.708629124	-1.486783109

Coord_9

C	2.055276148	2.116950153	0.792799056
N	0.711659049	1.953766140	0.557736040
C	0.366281024	0.888169063	-0.152176010
C	2.659637191	0.610036046	-0.799325055
N	3.030746216	1.473322104	0.199803015
N	1.356788098	0.134246008	-0.634748047
H	3.386721244	-0.043259002	-1.245411088
N	-0.896224066	0.532679037	-0.360877024

H	-1.075445076	-0.356347028	-0.785731058
H	-1.641807118	1.037568077	0.081816005
H	2.328193170	2.875803208	1.509507107
O	-1.161061081	3.884299282	1.907325137
H	-0.497588034	3.326163242	1.508087107
H	-0.941339068	4.778636344	1.683112123
O	-3.153908226	2.179937158	0.756079055
H	-3.912408283	1.952029142	1.276086091
H	-2.693485193	2.880447209	1.213923089
O	-0.739603053	-2.524115183	-1.179386087
H	0.188417015	-2.676245191	-1.328601096
H	-1.071716075	-3.278093235	-0.710048054
O	4.851827347	3.695931268	2.924049208
H	5.156278370	3.647906263	3.819575274
H	5.325889383	3.029511217	2.436380178
O	5.818698418	1.578909116	1.127865084
H	4.931569353	1.545094113	0.774312058
H	6.396212463	1.764059128	0.400149029
O	1.865873133	-2.601524189	-1.764400125
H	2.184398159	-2.562078184	-2.657513190
H	1.701428122	-1.708893125	-1.486894109

Coord_10

C	2.036715145	2.118517152	0.743930056
N	0.686605052	1.995646143	0.532741041
C	0.315451025	0.960504068	-0.204825013
C	2.591971185	0.714465054	-0.949486069
N	2.995698215	1.504382110	0.101718006
N	1.300239095	0.225188018	-0.725457055
H	3.289289234	0.057686004	-1.435800104
N	-0.951704068	0.616501047	-0.403698031
H	-1.142876080	-0.257077017	-0.854064060
H	-1.685431120	1.103268078	0.077084006
H	2.334283169	2.839158202	1.490787107
O	-1.142089082	3.870173276	1.961443142
H	-0.495685034	3.319576239	1.523747108
H	-0.925355068	4.769077345	1.753469127
O	-3.183215231	2.222876161	0.819226057
H	-3.923897282	1.981517142	1.358319098
H	-2.700484192	2.903183209	1.284867094
O	-0.756807055	-2.405244172	-1.334464094
H	0.170740013	-2.536104181	-1.504013109
H	-1.072007075	-3.188468231	-0.902935066
O	4.878645352	3.621721261	2.887091210
H	5.199803373	3.544917253	3.774676272
H	5.333864386	2.963212214	2.371416172
O	5.791491415	1.552241112	1.006956073

H	4.900191354	1.538340113	0.661959050
H	6.361237456	1.770437127	0.282273019
O	2.293415165	-2.555388183	-1.654684118
H	2.835968205	-3.228916233	-2.045995146
H	2.653949192	-2.369708173	-0.797194058

LIIC path connecting S2-MIN and S₁/S₀

Coord_1

C	2.036715145	2.118517152	0.743930056
N	0.686605052	1.995646143	0.532741041
C	0.315451025	0.960504068	-0.204825013
C	2.591971185	0.714465054	-0.949486069
N	2.995698215	1.504382110	0.101718006
N	1.300239095	0.225188018	-0.725457055
H	3.289289234	0.057686004	-1.435800104
N	-0.951704068	0.616501047	-0.403698031
H	-1.142876080	-0.257077017	-0.854064060
H	-1.685431120	1.103268078	0.077084006
H	2.334283169	2.839158202	1.490787107
O	-1.142089082	3.870173276	1.961443142
H	-0.495685034	3.319576239	1.523747108
H	-0.925355068	4.769077345	1.753469127
O	-3.183215231	2.222876161	0.819226057
H	-3.923897282	1.981517142	1.358319098
H	-2.700484192	2.903183209	1.284867094
O	-0.756807055	-2.405244172	-1.334464094
H	0.170740013	-2.536104181	-1.504013109
H	-1.072007075	-3.188468231	-0.902935066
O	4.878645352	3.621721261	2.887091210
H	5.199803373	3.544917253	3.774676272
H	5.333864386	2.963212214	2.371416172
O	5.791491415	1.552241112	1.006956073
H	4.900191354	1.538340113	0.661959050
H	6.361237456	1.770437127	0.282273019
O	2.293415165	-2.555388183	-1.654684118
H	2.835968205	-3.228916233	-2.045995146
H	2.653949192	-2.369708173	-0.797194058

Coord_2

C	2.047597146	2.126931155	0.751383052
N	0.706574053	1.996100145	0.535250039
C	0.362512028	0.947893071	-0.200867016
C	2.626847188	0.739464054	-0.970650068
N	3.012139217	1.496351110	0.121918009
N	1.353265095	0.213205016	-0.720134050
H	3.340223243	0.103526009	-1.462738104
N	-0.902626063	0.586787040	-0.390740030

H	-1.101089080	-0.286593021	-0.844134059
H	-1.646146118	1.073231078	0.077217004
H	2.345851169	2.852683205	1.493455108
O	-1.163887084	3.859675278	1.967856140
H	-0.504851034	3.319107240	1.536744109
H	-0.957496071	4.762112340	1.764759129
O	-3.159655228	2.184003160	0.791237057
H	-3.909554282	1.936984141	1.314602093
H	-2.695492193	2.871915205	1.264910090
O	-0.824801061	-2.431345173	-1.332118098
H	0.095591007	-2.590504184	-1.508786108
H	-1.162891082	-3.197126232	-0.886804066
O	4.884085352	3.626804262	2.873141208
H	5.192570372	3.560721258	3.766154269
H	5.348672385	2.964043213	2.371623170
O	5.817304417	1.532143108	1.034447074
H	4.928102353	1.499990108	0.685626047
H	6.391121460	1.722665122	0.305149023
O	2.200469161	-2.615715188	-1.652880121
H	2.780349200	-3.240953232	-2.073647150
H	2.557542183	-2.338374170	-0.824540060

Coord_3

C	2.056123149	2.134875154	0.758555054
N	0.724060053	1.996440141	0.537882040
C	0.405905028	0.935016066	-0.196408015
C	2.656275190	0.767871056	-0.991030071
N	3.025203217	1.488029110	0.141306010
N	1.403510099	0.202709013	-0.713638050
H	3.384315244	0.153988013	-1.490904108
N	-0.856403060	0.556741039	-0.375781026
H	-1.060939074	-0.317187023	-0.830634060
H	-1.608847118	1.043403076	0.079424007
H	2.355566170	2.865230204	1.496017109
O	-1.183654087	3.850329277	1.968889142
H	-0.513378038	3.318649237	1.544237110
H	-0.987324073	4.755619341	1.768588129
O	-3.136548228	2.146407153	0.765097056
H	-3.894724280	1.894898134	1.274070090
H	-2.689912194	2.842149207	1.244493087
O	-0.885148064	-2.452079179	-1.326342097
H	0.028292001	-2.637132187	-1.508145111
H	-1.243364088	-3.201350231	-0.868777061
O	4.886882350	3.629812259	2.858427207
H	5.184400373	3.574539256	3.755964268
H	5.360739388	2.963942214	2.370004168
O	5.839605423	1.512628110	1.059120075

H	4.951970358	1.461442107	0.709102049
H	6.415846463	1.676263119	0.325186024
O	2.115574154	-2.663103191	-1.647236117
H	2.726549199	-3.236847234	-2.099751151
H	2.467849179	-2.295354166	-0.857321061

Coord_4

C	2.061937150	2.142939153	0.765415054
N	0.738698054	1.997326143	0.540662041
C	0.445101033	0.922412064	-0.191410015
C	2.679281192	0.800076058	-1.010468074
N	3.034339219	1.479741109	0.159824012
N	1.450288103	0.194109015	-0.705987052
H	3.420513249	0.209523017	-1.520228111
N	-0.813464057	0.526929039	-0.358830028
H	-1.022331074	-0.348287024	-0.813743061
H	-1.573909116	1.014423071	0.083753005
H	2.363128171	2.877472206	1.498349108
O	-1.201011085	3.842524278	1.964995143
H	-0.520958036	3.318482239	1.546505111
H	-1.014215072	4.750006342	1.765544127
O	-3.114162225	2.110832155	0.741020052
H	-3.879800280	1.856065134	1.236978088
H	-2.683793196	2.814541204	1.223944087
O	-0.935955065	-2.468016177	-1.317161094
H	-0.028849003	-2.675958192	-1.502057106
H	-1.311359094	-3.202230232	-0.848988059
O	4.886877349	3.630381262	2.843412205
H	5.175509375	3.585871259	3.744516270
H	5.369837385	2.962659213	2.366672172
O	5.857929423	1.493643109	1.080626076
H	4.971232357	1.422684101	0.732376053
H	6.434678463	1.631350116	0.341752023
O	2.041158148	-2.697054192	-1.636997120
H	2.676410194	-3.215855233	-2.124023152
H	2.384884172	-2.240781164	-0.894148062

Coord_5

C	2.064775149	2.151818155	0.771983054
N	0.750207056	1.999564145	0.543723040
C	0.479654032	0.910750067	-0.185698012
C	2.694878194	0.836483061	-1.028742073
N	3.039025221	1.471860104	0.177450012
N	1.492930106	0.187870015	-0.697064049
H	3.447706249	0.270583017	-1.550567113
N	-0.774108055	0.498011037	-0.339836026
H	-0.984907072	-0.379212026	-0.793651058

H	-1.541610110	0.987011070	0.090267008
H	2.368379171	2.890201211	1.500342106
O	-1.215595088	3.836631276	1.956761140
H	-0.527280037	3.318864236	1.543999113
H	-1.037555075	4.745661341	1.756403124
O	-3.092714222	2.078091149	0.719170053
H	-3.865147278	1.821357134	1.203461086
H	-2.677158191	2.789784203	1.203598084
O	-0.975170068	-2.479693177	-1.304798095
H	-0.073308004	-2.706966196	-1.490607108
H	-1.364721100	-3.200836231	-0.827818059
O	4.883787351	3.628298262	2.828439204
H	5.165961372	3.594434257	3.732115271
H	5.375635389	2.960067213	2.361666171
O	5.871780421	1.475164107	1.098632078
H	4.985339360	1.383701100	0.755433057
H	6.446871464	1.588019114	0.354243025
O	1.979848143	-2.717123197	-1.621224118
H	2.631857190	-3.176859231	-2.145966153
H	2.308520164	-2.174830158	-0.933268067

Coord_6

C	2.064414150	2.162306157	0.778322058
N	0.758331054	2.004088144	0.547298040
C	0.509170036	0.900811065	-0.178936011
C	2.702020193	0.877456065	-1.045556076
N	3.038717219	1.464781104	0.194191016
N	1.530752108	0.184467014	-0.686587049
H	3.464678249	0.337541027	-1.581673115
N	-0.738525055	0.470723034	-0.318694024
H	-0.948016067	-0.409169030	-0.770562054
H	-1.512134107	0.961963068	0.099033009
H	2.371252169	2.904322210	1.501877107
O	-1.227042087	3.832981275	1.944890139
H	-0.532018037	3.320005238	1.537329109
H	-1.056697078	4.742935343	1.742107126
O	-3.072357223	2.049071148	0.699622050
H	-3.851106279	1.791738131	1.173485084
H	-2.669988194	2.768620198	1.183752085
O	-1.000470074	-2.487514178	-1.289691095
H	-0.102262006	-2.730078197	-1.473969108
H	-1.401095098	-3.198093230	-0.805930060
O	4.877239349	3.623507261	2.813687202
H	5.155758369	3.600192261	3.718889269
H	5.377711389	2.956173214	2.354882172
O	5.880589423	1.457211107	1.112765080
H	4.993704361	1.344475096	0.778256053

H	6.451570462	1.546353110	0.361996027
O	1.934562139	-2.722929198	-1.598698117
H	2.594723187	-3.118347224	-2.164774155
H	2.238494160	-2.097793153	-0.972467073

Coord_7

C	2.060624151	2.175286155	0.784529058
N	0.762791055	2.011958143	0.551725042
C	0.533294036	0.893495062	-0.170590012
C	2.699558196	0.923254065	-1.060544075
N	3.032789216	1.458912105	0.210085014
N	1.563035111	0.184347012	-0.674070049
H	3.470075249	0.410611028	-1.613176116
N	-0.706791052	0.445882030	-0.295228019
H	-0.910659064	-0.437221034	-0.744695056
H	-1.485576108	0.940162066	0.110119007
H	2.371729170	2.920860211	1.502806109
O	-1.234956091	3.831845275	1.930225140
H	-0.534807039	3.322040242	1.527295109
H	-1.070912075	4.742126342	1.723802122
O	-3.053170219	2.024772143	0.682337047
H	-3.837977275	1.768302130	1.146805083
H	-2.662206193	2.751856196	1.164662085
O	-1.009059071	-2.491598178	-1.272540090
H	-0.112390009	-2.745005197	-1.452368103
H	-1.417717101	-3.194619229	-0.784339057
O	4.866737350	3.616125259	2.799108200
H	5.144833372	3.603398260	3.704702265
H	5.375503386	2.951144210	2.346009171
O	5.883639426	1.439869106	1.122554081
H	4.995639361	1.304979095	0.800819060
H	6.447706463	1.506436106	0.364233029
O	1.908705136	-2.714119196	-1.567750112
H	2.566598184	-3.038285219	-2.179205157
H	2.174403154	-2.010172143	-1.008973074

Coord_8

C	2.053100150	2.191728158	0.790702059
N	0.763219053	2.024365148	0.557432038
C	0.551671039	0.889829065	-0.159908014
C	2.686193195	0.973953071	-1.073287076
N	3.020461217	1.454640105	0.225186018
N	1.588991112	0.187886012	-0.658768048
H	3.462363247	0.489714036	-1.644554120
N	-0.678888049	0.424405033	-0.269190022
H	-0.871392064	-0.462209032	-0.716278052
H	-1.461939105	0.922611067	0.123589008

H	2.369790169	2.940963210	1.502892106
O	-1.238851090	3.833429277	1.913804140
H	-0.535198037	3.325016239	1.514946107
H	-1.079300080	4.743470341	1.702908125
O	-3.035132217	2.006361146	0.667154046
H	-3.826013276	1.752339127	1.122935083
H	-2.653633194	2.740401196	1.146551084
O	-0.997316072	-2.491568179	-1.254332091
H	-0.099540008	-2.751003199	-1.426021104
H	-1.411046102	-3.190561228	-0.764531053
O	4.851604352	3.606492259	2.784329200
H	5.133023369	3.604690257	3.689027268
H	5.368236385	2.945354212	2.334427169
O	5.879972423	1.423304101	1.127384083
H	4.990275361	1.265181092	0.823091062
H	6.433870462	1.468334106	0.360016026
O	1.906516136	-2.690214195	-1.525960111
H	2.548609184	-2.933581209	-2.187329155
H	2.115645154	-1.912831136	-1.039315076

Coord_9

C	2.041352145	2.212692160	0.796814056
N	0.759035055	2.042644147	0.564822041
C	0.563846042	0.890973062	-0.145934009
C	2.660391189	1.029280076	-1.083358075
N	3.000679217	1.452292103	0.239515016
N	1.607672117	0.195310014	-0.639656044
H	3.439761245	0.574226039	-1.675132119
N	-0.654773045	0.407343030	-0.240241015
H	-0.828157061	-0.482637036	-0.685510052
H	-1.441189102	0.910492066	0.139514010
H	2.365312171	2.965943213	1.501625107
O	-1.238061091	3.837921277	1.896886137
H	-0.532591040	3.328915239	1.501586107
H	-1.080659076	4.747188341	1.681152119
O	-3.018109215	1.995288144	0.653815049
H	-3.815400277	1.745485123	1.101180077
H	-2.643942191	2.735374198	1.129634081
O	-0.960070069	-2.486269178	-1.236297090
H	-0.057981004	-2.746421196	-1.394963098
H	-1.375946098	-3.185475231	-0.748644051
O	4.830852349	3.595286259	2.768460201
H	5.119987368	3.605288259	3.670701267
H	5.354772386	2.939478212	2.319027169
O	5.868228424	1.407793101	1.126403083
H	4.976436360	1.225040087	0.845031063
H	6.408082459	1.432080104	0.348152025

O	1.933801139	-2.650196193	-1.469539106
H	2.540864183	-2.798286202	-2.186017155
H	2.061164149	-1.807231128	-1.059153074

Coord_10

C	2.031688146	2.264279163	0.855384061
N	0.756042055	2.101385150	0.623201045
C	0.572282043	0.942881069	-0.096529005
C	2.625108190	1.140427085	-1.054436078
N	2.976781213	1.482141108	0.294716019
N	1.619009115	0.255062016	-0.594017041
H	3.404056244	0.721336050	-1.673898120
N	-0.632993046	0.446297032	-0.185591013
H	-0.778891056	-0.438519031	-0.643937046
H	-1.420302100	0.952789066	0.187484012
H	2.367134170	3.010282218	1.562671111
O	-1.219495088	3.865492280	1.955738140
H	-0.515543040	3.357187242	1.556284111
H	-1.057741076	4.776184343	1.749504124
O	-2.995314217	2.039110148	0.686934052
H	-3.800974275	1.791770130	1.121160080
H	-2.623802191	2.775198199	1.170816083
O	-0.896030065	-2.405912173	-1.241652088
H	0.013506000	-2.661313191	-1.383723098
H	-1.313764093	-3.116905226	-0.773223054
O	4.812966348	3.568537259	2.825701203
H	5.114213367	3.577260259	3.724006270
H	5.341484385	2.924589212	2.364425169
O	5.850140421	1.400177103	1.161846084
H	4.955701359	1.198042088	0.906002066
H	6.372034460	1.414289101	0.371180025
O	1.992265145	-2.531771182	-1.412996104
H	2.532767184	-2.547615183	-2.190398156
H	2.003736146	-1.641610116	-1.070561077

LIIC path connecting S₂/S₁ and T1-MIN

Coord_1

C	2.060445146	2.282308163	0.775020055
N	0.748986053	1.894929139	0.530101039
C	0.484232034	0.790414060	-0.192116012
C	2.733902196	0.476579036	-0.460365035
N	3.059404218	1.543423109	0.279551021
N	1.459598104	0.044074004	-0.720645050
H	3.538865254	-0.102917006	-0.878035064
N	-0.779972054	0.433360029	-0.386366026
H	-0.964289067	-0.450938033	-0.826183060
H	-1.534823111	0.969351071	0.004144003

H	2.262306163	3.121963224	1.411395100
O	-1.224910090	3.930384281	2.028615145
H	-0.507626035	3.414655246	1.683714120
H	-1.007725073	4.841864347	1.881828134
O	-3.031892219	2.117598151	0.691950049
H	-3.844069275	1.865938137	1.111465082
H	-2.666964190	2.844367206	1.190400086
O	-1.072698075	-2.573787184	-1.307675094
H	-0.172309013	-2.824868204	-1.497719107
H	-1.433421103	-3.250974235	-0.750194054
O	4.835406347	3.711157270	2.904373207
H	5.119665369	3.611883258	3.802531274
H	5.365238384	3.115043226	2.384304173
O	5.902844427	1.719795124	1.041696078
H	5.003443360	1.669064118	0.729622050
H	6.456185465	1.827653131	0.280503022
O	1.866502134	-2.603386189	-1.765776128
H	2.184240157	-2.562330184	-2.657024193
H	1.700955122	-1.706777125	-1.486005107

Coord_2

C	2.075047152	2.260366162	0.798691058
N	0.754320054	1.900569136	0.535193037
C	0.488375037	0.778709056	-0.177638013
C	2.734658194	0.504473038	-0.511577036
N	3.066689221	1.546276110	0.268632020
N	1.456181106	0.057709002	-0.736695054
H	3.537659253	-0.061135006	-0.951274069
N	-0.777140056	0.394370027	-0.319988021
H	-0.955692069	-0.486235034	-0.769497053
H	-1.525763109	0.951291066	0.052021002
H	2.283971166	3.075510220	1.464561104
O	-1.221707086	3.946171284	2.008192147
H	-0.506218037	3.441932248	1.642881121
H	-1.012923075	4.861892351	1.876585135
O	-3.039020220	2.127261155	0.692968048
H	-3.853946278	1.882196134	1.111096081
H	-2.673642195	2.856688204	1.186982083
O	-1.076965080	-2.580389183	-1.297886093
H	-0.176474014	-2.824666201	-1.496050108
H	-1.434133105	-3.270718235	-0.754366056
O	4.816581348	3.708936265	2.905982208
H	5.104756366	3.623080262	3.804289274
H	5.353948388	3.115639223	2.390337174
O	5.904167423	1.718979122	1.057081075
H	5.010165361	1.667033120	0.729989050
H	6.471582464	1.817991132	0.305102022

O	1.856517136	-2.595557186	-1.777597128
H	2.167048157	-2.558162183	-2.671517194
H	1.694724124	-1.697794124	-1.499601110

Coord_3

C	2.090432149	2.237800160	0.820101057
N	0.761066053	1.906969138	0.538563038
C	0.493701037	0.767668053	-0.163857010
C	2.733746195	0.534728038	-0.563001042
N	3.074235220	1.549436113	0.256669016
N	1.452743105	0.072043006	-0.753118054
H	3.533741257	-0.017088001	-1.024947073
N	-0.770976056	0.357334028	-0.252264018
H	-0.946457069	-0.519509038	-0.710269049
H	-1.514606111	0.933138069	0.099835008
H	2.305949167	3.026969219	1.515138109
O	-1.219773086	3.959787284	1.988590141
H	-0.505938039	3.467276250	1.604252113
H	-1.018480072	4.879336351	1.873198136
O	-3.044524219	2.135432155	0.690309049
H	-3.863083280	1.896748138	1.105055078
H	-2.679775195	2.867271209	1.181002084
O	-1.079856076	-2.588141185	-1.287779093
H	-0.179223015	-2.825213201	-1.493784108
H	-1.433262101	-3.291163236	-0.758226054
O	4.796666345	3.705896269	2.906094208
H	5.087883364	3.633836261	3.804648274
H	5.341744386	3.115192227	2.395478174
O	5.905140426	1.716616123	1.072527077
H	5.016996362	1.663458120	0.730007053
H	6.486922466	1.806044131	0.330393022
O	1.847724131	-2.587402184	-1.788478129
H	2.151162155	-2.553897184	-2.684966191
H	1.689260120	-1.688408123	-1.512700110

Coord_4

C	2.106267154	2.214772160	0.839407062
N	0.768961055	1.914413138	0.540146040
C	0.500016037	0.757526053	-0.150717010
C	2.730892199	0.567648043	-0.614501042
N	3.081757220	1.553087113	0.243811020
N	1.449082103	0.087340006	-0.769879056
H	3.526837256	0.029614002	-1.098967079
N	-0.761458057	0.322398022	-0.183079014
H	-0.936488068	-0.550703042	-0.648368048
H	-1.501556108	0.914896065	0.147589011
H	2.327751170	2.976361215	1.563379113

O	-1.218752086	3.971867284	1.968898143
H	-0.506338038	3.491243249	1.566998114
H	-1.024171071	4.894793354	1.870391137
O	-3.048252220	2.142278153	0.683779049
H	-3.871247278	1.909857139	1.093302078
H	-2.685154192	2.876447206	1.172000085
O	-1.081415079	-2.596819189	-1.277419094
H	-0.180594013	-2.826247203	-1.491003107
H	-1.430803104	-3.312136240	-0.761847055
O	4.775820344	3.701737269	2.904956207
H	5.069273364	3.643716264	3.803815275
H	5.328662383	3.113384224	2.399881172
O	5.905493425	1.712448122	1.088033076
H	5.023657360	1.658196119	0.729754053
H	6.501849466	1.791529127	0.356369026
O	1.840071133	-2.578587186	-1.798498132
H	2.136540152	-2.549160185	-2.697442196
H	1.684466123	-1.678307119	-1.525340111

Coord_5

C	2.122205153	2.191404159	0.856801060
N	0.777749054	1.923153141	0.539933041
C	0.507128036	0.748497056	-0.138099011
C	2.725799196	0.603561044	-0.665887048
N	3.088959222	1.557408110	0.230238015
N	1.444988102	0.103852009	-0.786890057
H	3.516640254	0.079395008	-1.173202085
N	-0.748544053	0.289761020	-0.112290010
H	-0.925750067	-0.579651043	-0.583649040
H	-1.486826104	0.896567063	0.195283016
H	2.348847170	2.923660210	1.609546113
O	-1.218293088	3.982911287	1.948246138
H	-0.507001034	3.514236254	1.530295110
H	-1.029768073	4.908743355	1.866953136
O	-3.050047221	2.147900153	0.673207051
H	-3.878191280	1.921715139	1.075811076
H	-2.689561196	2.884459209	1.159551085
O	-1.081705079	-2.606195189	-1.266820092
H	-0.180655011	-2.827499205	-1.487750106
H	-1.426770101	-3.333459241	-0.765258053
O	4.754215344	3.696194264	2.902799206
H	5.049197364	3.652322263	3.801974272
H	5.314748382	3.109932226	2.403674172
O	5.904960427	1.706252123	1.103551077
H	5.029856364	1.651129121	0.729287054
H	6.515984468	1.774191126	0.382958029
O	1.833467133	-2.568778182	-1.807717130

H	2.123094155	-2.543565183	-2.709007195
H	1.680211120	-1.667179120	-1.537530112

Coord_6

C	2.137895152	2.167780157	0.872513063
N	0.787193058	1.933401140	0.537988040
C	0.514856035	0.740775053	-0.125816008
C	2.718149198	0.642811046	-0.716916049
N	3.095544225	1.562566112	0.216160016
N	1.440245102	0.121822011	-0.804005056
H	3.502804253	0.132714008	-1.247477092
N	-0.732176055	0.259686020	-0.039735004
H	-0.914291067	-0.606070042	-0.515959036
H	-1.470632106	0.878154066	0.242921018
H	2.368683173	2.868787207	1.653914117
O	-1.218049090	3.993301286	1.925801138
H	-0.507533037	3.536527253	1.493334106
H	-1.035032074	4.921565352	1.861741131
O	-3.049753221	2.152343157	0.658444048
H	-3.883662279	1.932441138	1.052564076
H	-2.692775196	2.891474210	1.143258082
O	-1.080808076	-2.616043188	-1.255948092
H	-0.179495013	-2.828703205	-1.484037107
H	-1.421189102	-3.354958242	-0.768448055
O	4.732037340	3.689032263	2.899845207
H	5.027973361	3.659292263	3.799301276
H	5.300064380	3.104590224	2.406958171
O	5.903288422	1.697844121	1.118985082
H	5.035299365	1.642162117	0.728633055
H	6.528938468	1.753817125	0.410012031
O	1.827790130	-2.557639186	-1.816186130
H	2.110691150	-2.536713184	-2.719714197
H	1.676343120	-1.654712122	-1.549253113

Coord_7

C	2.152993156	2.143938155	0.886815062
N	0.797079058	1.945328139	0.534454040
C	0.523038036	0.734533053	-0.113605010
C	2.707600198	0.685770047	-0.767279055
N	3.101213221	1.568721115	0.201821017
N	1.434642105	0.141481009	-0.821018057
H	3.484939250	0.190078012	-1.321573093
N	-0.712294051	0.232505015	0.034759002
H	-0.902271065	-0.629548044	-0.445133033
H	-1.453195107	0.859657061	0.290501021
H	2.386691170	2.811603202	1.696772124
O	-1.217669087	4.003316288	1.900756137

H	-0.507564036	3.558273258	1.455313107
H	-1.039704074	4.933556355	1.853660134
O	-3.047210217	2.155593157	0.639351047
H	-3.887403282	1.942093141	1.023541075
H	-2.694571192	2.897592208	1.122745082
O	-1.078821079	-2.626137191	-1.244723089
H	-0.177227012	-2.829585206	-1.479844108
H	-1.414094099	-3.376463243	-0.771377056
O	4.709486340	3.680029265	2.896324209
H	5.005963360	3.664280262	3.795974275
H	5.284692379	3.097140223	2.409818173
O	5.900247426	1.687083122	1.134185079
H	5.039697362	1.631234120	0.727793055
H	6.540321472	1.730250126	0.437301029
O	1.822885133	-2.544827181	-1.823950134
H	2.099150149	-2.528183180	-2.729617199
H	1.672689120	-1.640593117	-1.560466114

Coord_8

C	2.167168158	2.119870153	0.900026067
N	0.807225058	1.959069141	0.529559040
C	0.531537041	0.729922051	-0.101127005
C	2.693781194	0.732843052	-0.816590061
N	3.105675222	1.576029111	0.187500014
N	1.427975101	0.163056010	-0.837653062
H	3.462599250	0.252053019	-1.395212103
N	-0.688851049	0.208631014	0.111364008
H	-0.889989062	-0.649532047	-0.370989029
H	-1.434739103	0.841073060	0.338023022
H	2.402297173	2.751903197	1.738427126
O	-1.216802089	4.013153291	1.872302133
H	-0.506735038	3.579528260	1.415422101
H	-1.043502075	4.944941355	1.841623130
O	-3.042258219	2.157589156	0.615779043
H	-3.889162278	1.950682142	0.988696071
H	-2.694717192	2.902853209	1.097622080
O	-1.075855078	-2.636243191	-1.233030087
H	-0.173987013	-2.829863204	-1.475131107
H	-1.405534102	-3.397797246	-0.773983058
O	4.686780339	3.668971265	2.892482208
H	4.983571357	3.666942261	3.792182271
H	5.268737378	3.087385222	2.412328172
O	5.895638424	1.673878123	1.148948082
H	5.042769363	1.618316115	0.726728054
H	6.549751469	1.703396122	0.464508032
O	1.818563131	-2.529990183	-1.831053132
H	2.088242149	-2.517526180	-2.738773198

H 1.669054122 -1.624501117 -1.571103111

Coord_9

C 2.180111156 2.095525152 0.912510068
N 0.817492059 1.974724141 0.523621036
C 0.540246039 0.727086053 -0.087962007
C 2.676284192 0.784482057 -0.864375063
N 3.108642224 1.584650112 0.173517014
N 1.420050101 0.186779016 -0.853560061
H 3.435267245 0.319282025 -1.468041106
N -0.661839048 0.188566015 0.190244015
H -0.877914063 -0.665304048 -0.293312022
H -1.415500102 0.822399062 0.385483030
H 2.414935175 2.689417191 1.779198127
O -1.215087089 4.022935291 1.839597133
H -0.504689037 3.600246259 1.372828101
H -1.046104076 4.955882359 1.824511131
O -3.034736218 2.158223158 0.587540044
H -3.888691278 1.958175139 0.947923070
H -2.692976194 2.907251212 1.067461078
O -1.072042075 -2.646105192 -1.220718090
H -0.169941014 -2.829229202 -1.469839107
H -1.395581098 -3.418760248 -0.776190056
O 4.664158335 3.655630262 2.888594210
H 4.961255355 3.666916263 3.788144272
H 5.252331380 3.075140219 2.414559173
O 5.889299426 1.658180122 1.163010084
H 5.044248361 1.603421114 0.725363052
H 6.556869475 1.673228118 0.491216036
O 1.814594132 -2.512756182 -1.837533130
H 2.077681147 -2.504256182 -2.747241199
H 1.665217121 -1.606099116 -1.581073112

Coord_10

C 2.407829171 2.029857145 0.980960071
N 1.038863074 1.949059140 0.591667044
C 0.752902055 0.679947049 0.010798999
C 2.847250206 0.791590055 -0.853764064
N 3.316175238 1.550415112 0.206815016
N 1.604170117 0.163116014 -0.792671059
H 3.586759261 0.340098027 -1.490943109
N -0.422672030 0.127998007 0.374079027
H -0.664090047 -0.723259054 -0.102092008
H -1.185118088 0.759254055 0.542419037
H 2.651867191 2.587215189 1.869896134
O -0.984758071 3.994929289 1.893237137
H -0.279822018 3.580436259 1.410837103

H	-0.820116059	4.928731354	1.885988133
O	-2.812620201	2.113047153	0.678807048
H	-3.669201266	1.921617140	1.037650073
H	-2.471278179	2.868816206	1.148115083
O	-0.877262063	-2.707545195	-1.085605078
H	0.021603000	-2.880417205	-1.352890099
H	-1.188104087	-3.489250251	-0.648025046
O	4.883151354	3.608940260	2.901336211
H	5.192565372	3.637391263	3.796362273
H	5.470909392	3.027340220	2.427970175
O	6.100546439	1.601362117	1.185884088
H	5.257464378	1.545553111	0.744722054
H	6.772052487	1.598207115	0.517874039
O	1.992320142	-2.547043185	-1.759953126
H	2.236736159	-2.546465185	-2.674907193
H	1.845557134	-1.638177116	-1.509195109