

Supporting Information: Photophysics of Auramine-O: Electronic Structure Calculations and Nonadiabatic Dynamics Simulations

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Table of Contents

1. Active Orbitals in OM2/MRCI and CASSCF Calculations
2. Three Dihedral Angles of All Optimized Structures at OM2/MRCI and SA-CASSCF Level
3. Computed Vertical Excitation Energies to the S₁ State
4. Cartesian Coordinates of All Optimized Structures and LIIC Paths

1. Active Orbitals in OM2/MRCI and CASSCF Calculations

1.1 OM2/MRCI (12, 12) for the $^1\pi\pi^*$ state

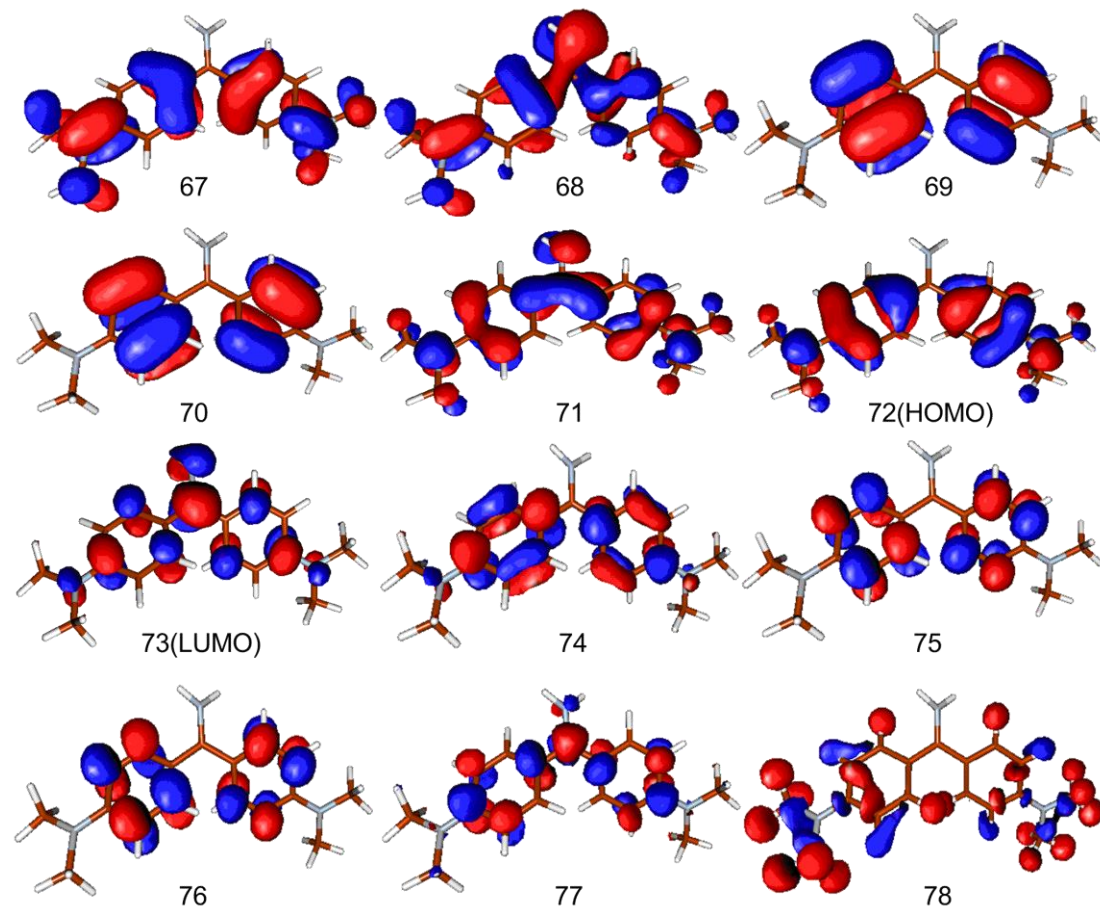


Fig. S1: Molecular orbitals (6 highest occupied and 6 lowest unoccupied) used in the active space (12, 12) of the OM2/MRCI calculations. See text for simulation details.

1.2 CASSCF (10, 8) for the $^1\pi\pi^*$ state

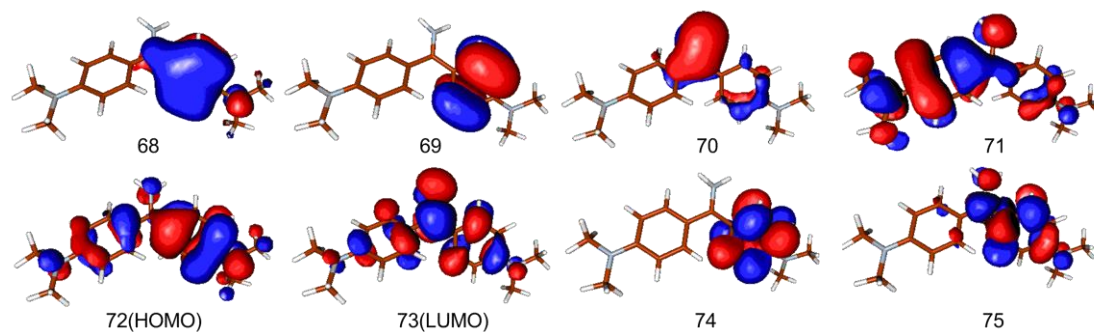


Fig. S2: Molecular orbitals (5 highest occupied and 3 lowest unoccupied) used in the active space (10, 8) of the CASSCF calculations.

2. Three Dihedral Angles of All optimized Structures at OM2/MRCI and SA-CASSCF Level

Table S1: Selected Dihedral Angles (in degree) of OM2/MRCI [SA-CASSCF] Method Based on Optimized Structures.

	ϕ_1	ϕ_2	ϕ_3
S0	28.6[29.8]	28.6[29.2]	179.9[179.9]
S1-LE	30.5[27.8]	30.5[28.3]	180.0[177.7]
S1-I1	32.6[19.5]	103.6[101.1]	145.0[154.6]
S1-I2	74.6[77.2]	31.6[19.6]	145.1[152.8]
S1-II	127.8[128.1]	33.9[34.9]	137.0[138.9]
S1S0-I1	18.5[16.0]	97.5[98.8]	156.7[149.4]
S1S0-I2	97.3[98.1]	19.0[16.3]	156.2[146.4]
S1S0-II	135.6[162.7]	48.7[34.2]	128.8[117.5]

3. Computed Vertical Excitation Energies to the S₁ State

Table S2: Computed Vertical Excitation Energies (unit: eV) to the S₁ State. Experimental Value in Methanol.

B3LYP-Gas	CAM-B3LYP-Gas	CAM-B3LYP-Methanol	Exp.
3.00	3.30	3.33	3.00

4. Cartesian Coordinates of Optimized Structures and Paths

In xyz format (unit: angström)

4.1 OM2/MRCI Method

S0

C -0.704422700 2.599434800 -0.964831800

C	-0.676351200	1.394693000	-0.289003300
C	-0.070265100	1.310815100	0.985468600
C	0.500290800	2.464820000	1.570436600
C	0.504336800	3.663010700	0.887017300
C	-0.103891800	3.759808800	-0.398921800
H	-1.157282600	0.5144416200	-0.727779000
H	0.988385500	2.409114900	2.552830900
H	0.962790000	4.541005900	1.343552100
C	-0.099144800	0.050991700	1.704895500
C	-0.084490400	-1.219607300	1.004161000
C	0.598891300	-1.322631900	-0.229169000
C	-0.690782000	-2.364769900	1.570285800
C	0.667934100	-2.537473900	-0.883527000
H	1.106410800	-0.448947800	-0.650811700
C	-0.653369500	-3.573202500	0.906267600
H	-1.238546900	-2.294235000	2.519693100
C	0.033071600	-3.689468400	-0.338089100
H	1.199928800	-2.602410000	-1.833163500
H	-1.139645500	-4.444309900	1.346909500
N	-0.140031600	0.061002400	3.039608200
H	-0.120723000	-0.782313600	3.581016400

H	-0.192003100	0.912318600	3.566131700
N	0.069218700	-4.895826100	-1.005199800
C	0.758802100	-5.007313200	-2.267738100
H	0.695776700	-6.046742000	-2.650056700
H	0.321325000	-4.328455100	-3.033848200
H	1.846639400	-4.768603600	-2.160526500
C	-0.563507200	-6.065846200	-0.440705000
H	-0.122472700	-6.327230700	0.548840500
H	-1.657823500	-5.903730400	-0.311073500
H	-0.432495700	-6.935098500	-1.112954700
H	-1.176914600	2.649577000	-1.946315400
N	-0.098134500	4.955904300	-1.085469600
C	-0.708096800	5.047568600	-2.389866400
H	-0.621098500	6.081052900	-2.783437200
H	-0.224240900	4.357270300	-3.116863300
H	-1.800577900	4.809902000	-2.346662600
C	0.499328900	6.134587000	-0.501070300
H	-0.001532900	6.410953700	0.455317100
H	1.583545000	5.974876200	-0.301943800
H	0.410463600	6.993393800	-1.193375800

S1-LE

C	-0.693560800	2.601219700	-0.974883200
C	-0.700093900	1.406467600	-0.275935100
C	-0.082116000	1.315064900	0.990925800
C	0.515530700	2.461133900	1.561988700
C	0.495150600	3.670140500	0.889129700
C	-0.103701500	3.762540100	-0.400008000
H	-1.185117600	0.529212400	-0.710738700
H	1.006477100	2.397157000	2.537790800
H	0.943219400	4.551143100	1.353666500
C	-0.099582900	0.051074900	1.719886700
C	-0.072987300	-1.223767900	1.010456100
C	0.621832900	-1.334249300	-0.214454800
C	-0.705456700	-2.361252600	1.560856800
C	0.657683100	-2.539461200	-0.894144000
H	1.133150100	-0.463465900	-0.631818300
C	-0.644298800	-3.580300600	0.909085200
H	-1.255660900	-2.282538000	2.503428400
C	0.032998600	-3.692128800	-0.339094200
H	1.182935800	-2.603318300	-1.848541900
H	-1.120698800	-4.454307900	1.358400200

N	-0.141183100	0.061274600	3.073300000
H	-0.082420100	-0.777174000	3.607864700
H	-0.231882900	0.907634700	3.590611200
N	0.074705700	-4.903325500	-1.008071400
C	0.764307600	-5.023590100	-2.269692800
H	0.694475300	-6.058030200	-2.658173800
H	0.324515500	-4.343179100	-3.032944300
H	1.844552800	-4.777510000	-2.159665200
C	-0.564419900	-6.072955700	-0.452033700
H	-0.125437300	-6.332827300	0.537160400
H	-1.657511800	-5.906820700	-0.318894600
H	-0.436314500	-6.945045000	-1.120543000
H	-1.159025400	2.650266500	-1.960632600
N	-0.103395900	4.963255200	-1.088787200
C	-0.713478200	5.063829400	-2.392401300
H	-0.619307800	6.092229500	-2.791638400
H	-0.227508500	4.372037100	-3.116427200
H	-1.798565500	4.818859100	-2.345743400
C	0.500972400	6.141544100	-0.512440200
H	0.002089100	6.416347600	0.443780300
H	1.583704300	5.977865600	-0.309771500

H 0.414718900 7.003251900 -1.200823800

S1-I1

C 1.196742400 1.966002200 -1.129163000

C 0.826817300 0.979193700 -0.250784200

C 0.020005500 1.284458600 0.873612100

C -0.446252200 2.606676900 1.080357100

C -0.136087700 3.609029500 0.194353700

C 0.728461400 3.319678300 -0.919214200

H 1.145761900 -0.051313700 -0.396232300

H -1.080535800 2.809636300 1.942178600

H -0.520152600 4.622122100 0.350243500

C -0.311478200 0.224407200 1.871994600

C -1.231865400 -0.822185600 1.436091000

C -2.022125100 -0.647875300 0.287900700

C -1.485653300 -1.924251500 2.275420200

C -2.998618900 -1.570321600 -0.050655800

H -1.856633200 0.218972500 -0.370560400

C -2.448300500 -2.861404700 1.941938600

H -0.919391500 -2.059281400 3.207082400

C -3.220707800 -2.706573800 0.767058600

H	-3.593746400	-1.420193200	-0.952320500
H	-2.612318600	-3.717049500	2.596490800
N	0.778012000	-0.060372300	2.671114800
H	0.766574200	-0.934156600	3.167028500
H	1.122585500	0.690518100	3.249722600
N	-4.169300500	-3.666043900	0.415922800
C	-5.019193400	-3.469885200	-0.725108500
H	-5.713174000	-4.328827800	-0.847285800
H	-5.642779500	-2.542574800	-0.626855300
H	-4.420457400	-3.385372300	-1.668057000
C	-4.423857500	-4.780734500	1.290873000
H	-3.496000200	-5.390326200	1.438011600
H	-4.778963000	-4.444535500	2.298399300
H	-5.198617600	-5.447126100	0.860007400
H	1.839082500	1.718406000	-1.967823700
N	1.106047600	4.315750100	-1.760662600
C	1.971390100	4.024563000	-2.902701900
H	2.170202100	4.949454100	-3.463434500
H	2.945739600	3.615091200	-2.555904100
H	1.480225500	3.307466100	-3.594787600
C	0.678022500	5.681300300	-1.548360800

H	-0.420516900	5.759528800	-1.600611900
H	1.026785300	6.056704900	-0.572533700
H	1.092273700	6.340963500	-2.324874400

S1-I2

C	-2.133793800	2.185776700	-0.565132100
C	-1.473406300	1.089054600	-0.035993800
C	-0.641057400	1.221738600	1.087998100
C	-0.439309100	2.502902400	1.637695000
C	-1.103841400	3.605131500	1.128467800
C	-1.971618900	3.466572300	0.019721600
H	-1.623519700	0.100549500	-0.496649100
H	0.248730500	2.646478900	2.482400700
H	-0.951926100	4.581539400	1.588296300
C	0.170817800	0.100160800	1.552943500
C	-0.190481400	-1.252352700	1.033320200
C	0.691891900	-1.913198000	0.143264800
C	-1.385965100	-1.884911000	1.457373400
C	0.400410800	-3.166800400	-0.334452500
H	1.592430300	-1.393762600	-0.182907300
C	-1.681872200	-3.158332900	1.042159100

H	-2.053122100	-1.338996100	2.120858300
C	-0.781852900	-3.839902200	0.136150400
H	1.074751200	-3.657616700	-1.042350800
H	-2.586117300	-3.638378200	1.400243200
N	0.618509400	0.025703900	2.856908300
H	1.456793600	-0.510930000	3.017606300
H	0.612908200	0.876532200	3.391219000
N	-1.045106100	-5.109719200	-0.266457300
C	-0.142703600	-5.823583800	-1.144295300
H	-0.521104500	-6.837959600	-1.343169900
H	-0.050526600	-5.305498700	-2.114503000
H	0.855385400	-5.924347900	-0.685185400
C	-2.256797000	-5.788363600	0.191544100
H	-2.250692700	-5.885276700	1.299343100
H	-3.164028000	-5.237004200	-0.137349800
H	-2.301995400	-6.798827800	-0.240684100
H	-2.786583600	2.056158700	-1.428403500
N	-2.662896000	4.571529900	-0.475527500
C	-3.480668100	4.454102200	-1.650775100
H	-3.952688000	5.429255200	-1.897251900
H	-2.883536400	4.131763200	-2.544044300

H	-4.304847000	3.710525700	-1.499211000
C	-2.437568800	5.875207500	0.092633100
H	-2.699468600	5.885948800	1.181636600
H	-1.368193100	6.192479100	-0.007262300
H	-3.067945300	6.636502600	-0.411061200

S1-II

C	-2.481032600	2.102430400	-0.038971300
C	-1.954425100	1.009202100	0.630164500
C	-0.746995000	1.119160500	1.340672800
C	-0.064405800	2.346280700	1.349203200
C	-0.582423400	3.451531900	0.693598000
C	-1.802113500	3.348406300	-0.027065100
H	-2.498371200	0.059167600	0.627552400
H	0.869440400	2.447726800	1.914811300
H	-0.054912800	4.404804600	0.737595400
C	-0.220996800	-0.060791600	2.071709700
C	0.412253300	-1.033945300	1.143638600
C	1.753604700	-0.866711600	0.716281400
C	-0.338744700	-2.120156200	0.633596100
C	2.336399700	-1.749638900	-0.166323000

H	2.336390100	-0.039704900	1.126165200
C	0.220037300	-3.015342100	-0.254711500
H	-1.374106800	-2.249214100	0.959182600
C	1.578135300	-2.850144900	-0.684559900
H	3.381498400	-1.625442300	-0.451387700
H	-0.372170100	-3.847192600	-0.638601800
N	0.448290300	0.167399500	3.243648600
H	0.893372400	-0.592713700	3.719367100
H	0.122610800	0.897795900	3.845432600
N	2.145848000	-3.731863000	-1.567691100
C	3.520223900	-3.573548900	-2.003571900
H	3.798251200	-4.369982700	-2.719160800
H	3.662763000	-2.598234800	-2.512783200
H	4.216229500	-3.636766800	-1.139909500
C	1.385954300	-4.837758900	-2.115601100
H	1.049080000	-5.520904800	-1.308863700
H	0.498442600	-4.472086400	-2.675249200
H	2.003091800	-5.427770000	-2.818940700
H	-3.427462600	2.005132500	-0.573957100
N	-2.314016900	4.443783200	-0.708451000
C	-3.554232200	4.341756900	-1.436895000

H	-3.810238100	5.310333900	-1.914672000
H	-3.485974900	3.575980300	-2.247372900
H	-4.400656100	4.067201400	-0.761573200
C	-1.636783900	5.715160000	-0.674200300
H	-1.544718900	6.100686900	0.369777100
H	-0.612877400	5.640570500	-1.114761300
H	-2.194752600	6.476075800	-1.260577000

S1S0-I1

C	1.157333300	2.031064000	-1.272446500
C	0.860829300	0.983815500	-0.435434000
C	0.091607800	1.187463000	0.735138300
C	-0.428932300	2.471966900	1.027931700
C	-0.152701900	3.546402000	0.212780700
C	0.688384500	3.354688400	-0.948535700
H	1.221775000	-0.019738400	-0.655325000
H	-1.054246800	2.595653700	1.911797800
H	-0.568640400	4.543274400	0.433851100
C	-0.125019100	0.052721000	1.683514800
C	-1.135758800	-0.934325800	1.376924900
C	-2.054999100	-0.725206600	0.328042900
C	-1.282208200	-2.062695900	2.207237400
C	-3.059428600	-1.649954600	0.079466500

H	-1.980936500	0.173162000	-0.298382600
C	-2.265104300	-3.006712600	1.947843400
H	-0.596838900	-2.212655500	3.050268500
C	-3.151806400	-2.815476900	0.864161900
H	-3.764100600	-1.483297500	-0.740400900
H	-2.364424100	-3.898203500	2.568463900
N	0.978078400	-0.122259300	2.503016700
H	1.492286000	-0.982520400	2.350592600
H	0.756067200	-0.038181200	3.489977900
N	-4.089785800	-3.840323000	0.575738200
C	-4.492916600	-3.982469100	-0.796941400
H	-4.930868600	-4.993665700	-0.954756200
H	-5.272894700	-3.226743900	-1.100352300
H	-3.625579700	-3.876522100	-1.482780100
C	-5.151806500	-4.011952500	1.533997900
H	-4.778369700	-3.898309700	2.570852100
H	-5.977957300	-3.266363100	1.376366900
H	-5.595270000	-5.027304000	1.432315300
H	1.748989400	1.851197100	-2.160302400
N	1.037699300	4.417485100	-1.713949400
C	1.857546600	4.245783900	-2.903147300
H	1.986139300	5.208242900	-3.417604200
H	2.861460900	3.871395000	-2.633552400
H	1.372524700	3.552021600	-3.614842900
C	0.634713200	5.771975100	-1.336104100

H -0.470180200 5.860494800 -1.336878000

H 1.029908400 6.023536400 -0.329820500

H 1.040363100 6.506786300 -2.054535800

S1S0-I2

C -3.047969200 -1.658907500 -0.056560600

C -2.043677500 -0.733676000 -0.307134800

C -1.137562700 -0.936397900 -1.368150000

C -1.282625900 -2.064344200 -2.199142400

C -2.264965100 -3.007038700 -1.937394100

C -3.150132100 -2.814781900 -0.852878200

H -1.958604100 0.159363900 0.326798700

H -0.600883600 -2.210245600 -3.044859000

H -2.363571700 -3.900860800 -2.553824700

C -0.131898700 0.050932300 -1.682064900

C 0.086844700 1.185285300 -0.734544500

C 0.859570800 0.983388500 0.433702800

C -0.428800000 2.469713700 -1.036493100

C 1.155637700 2.034472900 1.266096500

H 1.217869700 -0.018668700 0.657569700

C -0.149171700 3.548769700 -0.228741100

H -1.047917000 2.588045600 -1.925971800

C 0.685712200 3.356308300 0.936902600

H 1.748551700 1.858661100 2.153068600

H -0.549927300 4.549678100 -0.464693300

N	0.970527100	-0.127566000	-2.500391400
N	-4.094960200	-3.835582000	-0.578559500
C	-4.499121000	-3.986037700	0.792050500
C	-5.149273400	-3.998438200	-1.546961100
N	1.031879500	4.416125100	1.707261000
C	1.859174400	4.246076100	2.893037000
C	0.624138400	5.773320100	1.347110900
H	1.477887400	-0.990786200	-2.346883800
H	0.748767400	-0.042339000	-3.486909800
H	-4.944236300	-4.994774300	0.942786900
H	-5.271748000	-3.225999800	1.102001500
H	-3.627722000	-3.891857100	1.475153200
H	-3.740119200	-1.497780500	0.773739700
H	-4.766616500	-3.880850400	-2.580661200
H	-5.974724400	-3.250507900	-1.394655900
H	-5.596775200	-5.013173300	-1.455364000
H	1.989593700	5.210905500	3.404725700
H	2.861822800	3.872977600	2.615965200
H	1.381356500	3.552885700	3.610099500
H	-0.480056500	5.859134000	1.341604900
H	1.025800300	6.041098500	0.349242300
H	1.022840100	6.497722900	2.079728900

S1S0-II

C	-2.544843800	1.992232300	0.199762000
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C	-2.081427800	0.954245800	0.979468700
C	-0.776609500	0.977079300	1.523669800
C	0.095355100	2.030987500	1.173647800
C	-0.353551900	3.094848500	0.418990200
C	-1.693187600	3.106696100	-0.081671200
H	-2.737284700	0.110374600	1.215033800
H	1.114239300	2.036452200	1.571688100
H	0.305806000	3.941998300	0.229062500
C	-0.373336300	-0.183659600	2.372871600
C	0.322145400	-0.976228000	1.314252400
C	1.640163600	-0.713780600	0.880569300
C	-0.430020500	-1.981037300	0.663668600
C	2.238586500	-1.511260000	-0.072699600
H	2.215761700	0.080893700	1.364806100
C	0.135175100	-2.771742100	-0.313484400
H	-1.466809300	-2.147056500	0.972818600
C	1.500459500	-2.569381600	-0.690427100
H	3.285095100	-1.353273700	-0.335158300
H	-0.452669300	-3.555590300	-0.791618600
N	0.288943100	0.060680200	3.558404900
H	0.682488000	-0.733636100	4.032935000
H	-0.127471700	0.727740200	4.184683500
N	2.088195600	-3.374545100	-1.633113500
C	3.469180500	-3.177981100	-2.021419500
H	3.781110700	-3.940183000	-2.760299900

H	3.615366400	-2.178699700	-2.485076500
H	4.142469300	-3.267703900	-1.139154000
C	1.342787500	-4.440032700	-2.270119100
H	0.913516400	-5.133433400	-1.515901100
H	0.514455300	-4.025291100	-2.889219400
H	1.997476500	-5.032156000	-2.938383300
H	-3.560862800	1.969007700	-0.194909400
N	-2.153345500	4.165160000	-0.824355400
C	-3.507786400	4.179484400	-1.335905400
H	-3.727239200	5.140488200	-1.840174300
H	-3.656035100	3.364821200	-2.081222100
H	-4.245055800	4.052177300	-0.514452100
C	-1.299185200	5.298076600	-1.111841100
H	-0.941693000	5.770873300	-0.169384500
H	-0.418549500	4.991495200	-1.716830700
H	-1.848733800	6.068244900	-1.686339900

4.2 CASSCF Method

S0

C	-0.68237929	2.69029657	-0.99310943
C	-0.65758398	1.46880595	-0.35370414
C	-0.06630470	1.30784417	0.91822595
C	0.50932742	2.46077434	1.50782155
C	0.50645663	3.67855638	0.86818142

C	-0.10109590	3.83897960	-0.41123438
H	-1.14374966	0.63740791	-0.82323665
H	1.01632142	2.38860966	2.45123237
H	0.98601857	4.50826437	1.33998950
C	-0.09012347	0.04418096	1.60918206
C	-0.07480284	-1.22840628	0.93807662
C	0.59701149	-1.40905099	-0.28914732
C	-0.69410947	-2.36481446	1.49956469
C	0.65880397	-2.62720398	-0.90590686
H	1.11175557	-0.58184074	-0.73520623
C	-0.65962583	-3.58497914	0.88681757
H	-1.25741674	-2.27261530	2.40885561
C	0.02877615	-3.76684518	-0.34307415
H	1.20821825	-2.71411341	-1.81746681
H	-1.17586631	-4.40352480	1.33841473
N	-0.13079375	0.05419228	2.94472682
H	0.02959290	-0.76949776	3.47572168
H	-0.31445093	0.88804785	3.45177218
N	0.07828957	-4.97219178	-0.94839720
C	0.76169848	-5.13470999	-2.23187933
H	0.65528627	-6.15443817	-2.56003331

H 0.33074976 -4.49317997 -2.99037420
H 1.81967454 -4.91793663 -2.14705882
C -0.54798996 -6.14413734 -0.33542880
H -0.13806032 -6.34010042 0.64741715
H -1.62112248 -6.02177532 -0.25183405
H -0.35790312 -7.00624739 -0.95143492
H -1.17052244 2.75922674 -1.94072575
N -0.11585566 5.03658875 -1.03366659
C -0.71474997 5.17711609 -2.36130860
H -0.59370961 6.19311378 -2.69593018
H -0.23086357 4.52870057 -3.08107536
H -1.77456939 4.95368138 -2.34292768
C 0.46203813 6.22118242 -0.39698760
H -0.01407346 6.42997553 0.55278426
H 1.52781280 6.10754556 -0.24015001
H 0.30918462 7.07282007 -1.03745697

S1-LE

C -0.679215000 2.695631000 -1.002046000
C -0.669050000 1.474509000 -0.338881000
C -0.075113000 1.324107000 0.932332000

C	0.493222000	2.498407000	1.516501000
C	0.485544000	3.697471000	0.880331000
C	-0.106830000	3.847252000	-0.416976000
H	-1.139342000	0.634554000	-0.808237000
H	0.959911000	2.421721000	2.478324000
H	0.938936000	4.539178000	1.356803000
C	-0.074306000	0.051547000	1.647692000
C	-0.065835000	-1.241935000	0.970907000
C	0.609954000	-1.429237000	-0.277755000
C	-0.675471000	-2.382160000	1.535574000
C	0.659175000	-2.631505000	-0.900104000
H	1.109565000	-0.595490000	-0.728263000
C	-0.634183000	-3.621248000	0.902670000
H	-1.203250000	-2.293411000	2.463618000
C	0.026987000	-3.788161000	-0.333358000
H	1.186330000	-2.713866000	-1.825856000
H	-1.120303000	-4.449376000	1.370550000
N	-0.132003000	0.073027000	3.036506000
H	0.269913000	-0.651592000	3.577650000
H	-0.584498000	0.805279000	3.525408000
N	0.068827000	-4.978502000	-0.968023000

C	0.775484000	-5.126852000	-2.241541000
H	0.688808000	-6.145602000	-2.576181000
H	0.349453000	-4.483430000	-3.001116000
H	1.827369000	-4.896216000	-2.131516000
C	-0.586244000	-6.157232000	-0.398053000
H	-0.160132000	-6.413458000	0.563839000
H	-1.649690000	-5.991101000	-0.280747000
H	-0.446303000	-6.992459000	-1.062184000
H	-1.135041000	2.749258000	-1.966561000
N	-0.109814000	5.037499000	-1.051753000
C	-0.731913000	5.179004000	-2.369325000
H	-0.632573000	6.198347000	-2.699904000
H	-0.250913000	4.537419000	-3.097559000
H	-1.786482000	4.937699000	-2.327345000
C	0.501299000	6.221924000	-0.444132000
H	0.014667000	6.477185000	0.488744000
H	1.556869000	6.065570000	-0.262210000
H	0.395486000	7.054549000	-1.117795000

S1-H1

C	1.25963839	2.01518775	-1.10777246
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C	0.89038971	1.04616135	-0.23499851
C	0.03947983	1.30417350	0.88828156
C	-0.42269959	2.63238984	1.06988793
C	-0.07389834	3.63569145	0.19795932
C	0.79432727	3.36503303	-0.93784786
H	1.25161012	0.04686277	-0.36983492
H	-1.06832105	2.84897893	1.89640209
H	-0.44599493	4.62411859	0.35559526
C	-0.29680571	0.21462720	1.82971528
C	-1.29882261	-0.78495343	1.46557744
C	-2.10008136	-0.65199926	0.34459744
C	-1.52650793	-1.92810482	2.27243118
C	-3.06798213	-1.59493455	0.00036838
H	-1.99890360	0.20293336	-0.29608051
C	-2.47864893	-2.86653552	1.94588069
H	-0.97084043	-2.06824004	3.17846531
C	-3.28234782	-2.72924353	0.78008101
H	-3.65001795	-1.42322247	-0.87965923
H	-2.61386953	-3.70494220	2.59523829
N	0.73436149	-0.09445123	2.72910571
H	0.87943697	-1.03313421	3.01138713

H	1.08047242	0.60055550	3.34645808
N	-4.22695352	-3.67192303	0.45601470
C	-5.04644581	-3.50140631	-0.73301414
H	-5.72089654	-4.33686091	-0.82404465
H	-5.64174105	-2.59547822	-0.68160688
H	-4.44030636	-3.46239429	-1.63212701
C	-4.43196414	-4.83967750	1.30147972
H	-3.53227261	-5.44019172	1.37969279
H	-4.74889957	-4.56232843	2.30116871
H	-5.20300943	-5.45661804	0.87014584
H	1.90961806	1.77403806	-1.91937887
N	1.13647936	4.32800811	-1.77088421
C	2.01130733	4.05679236	-2.92931313
H	2.14668754	4.96685111	-3.48412506
H	2.97920029	3.70744642	-2.59983154
H	1.56078607	3.32207359	-3.58038781
C	0.66842459	5.71747628	-1.58834185
H	-0.40888703	5.76902670	-1.65083734
H	0.99985148	6.11037282	-0.63835615
H	1.08306133	6.32735517	-2.36962351

S1-I2

C -2.09724075 2.25909148 -0.59068548

C -1.41923289 1.15495515 -0.07520153

C -0.58958648 1.24185790 1.02944204

C -0.43969684 2.52781568 1.60689718

C -1.10147907 3.62663848 1.10850440

C -1.96748239 3.52097239 -0.01517887

H -1.55731111 0.21668492 -0.57736422

H 0.22258729 2.67226163 2.43743735

H -0.94490053 4.57413266 1.57815525

C 0.13087210 0.08435453 1.55570219

C -0.16849350 -1.27056037 1.04478788

C 0.69329773 -1.94883609 0.14580844

C -1.34384927 -1.96136267 1.48484199

C 0.41030344 -3.21978795 -0.29355726

H 1.57315002 -1.44989380 -0.20599759

C -1.64674516 -3.21790340 1.07679723

H -1.99193717 -1.45779899 2.17306899

C -0.78381250 -3.91519224 0.16213627

H 1.07333599 -3.70054750 -0.97877954

H -2.52628415 -3.69522277 1.44816309

N	0.65853590	0.09509606	2.85545126
H	1.50600143	-0.38158261	3.05185021
H	0.42095555	0.82734392	3.47934085
N	-1.05284354	-5.13759631	-0.25213485
C	-0.15743550	-5.85949891	-1.17949725
H	-0.56177526	-6.83867670	-1.35839991
H	-0.08798151	-5.34101510	-2.12479965
H	0.82707262	-5.97190467	-0.74973402
C	-2.26864540	-5.84375925	0.19942232
H	-2.24793033	-5.98764655	1.27011168
H	-3.15336184	-5.28921045	-0.07684038
H	-2.30827398	-6.80704216	-0.27478993
H	-2.71925618	2.11482057	-1.44797896
N	-2.62995478	4.61990544	-0.50459312
C	-3.50126517	4.48828692	-1.66121976
H	-3.93681715	5.44687894	-1.89047171
H	-2.95568529	4.15109199	-2.53667238
H	-4.31062980	3.79077791	-1.47239370
C	-2.45761113	5.92735900	0.11286898
H	-2.76919332	5.92390935	1.15165628
H	-1.42730490	6.26308888	0.06347646

H -3.06468327 6.64756808 -0.41051734

S1-II

C -2.47145188 2.11865310 -0.04433476

C -1.95418225 1.03967129 0.63406346

C -0.75995512 1.12580640 1.35874861

C -0.09756097 2.36038402 1.35891272

C -0.60176703 3.45178057 0.68973355

C -1.80968505 3.36623674 -0.03806300

H -2.50003038 0.11571226 0.62236953

H 0.82372723 2.46213502 1.89927690

H -0.06305627 4.37392944 0.73200492

C -0.20529313 -0.05491670 2.06926191

C 0.40708349 -1.04755385 1.15220310

C 1.75228070 -0.88862652 0.71889831

C -0.33014071 -2.14043586 0.62333022

C 2.33910669 -1.76933327 -0.16167030

H 2.32460935 -0.06979855 1.10441115

C 0.22573045 -3.02451662 -0.26947253

H -1.34400747 -2.28486890 0.93751098

C 1.59231070 -2.87284249 -0.70390367

H	3.36095409	-1.63026109	-0.43937219
H	-0.36056883	-3.83835383	-0.63591283
N	0.48286756	0.17984127	3.26360962
H	0.88822269	-0.59155914	3.74018151
H	0.14253327	0.90115529	3.85663410
N	2.13817504	-3.71833175	-1.56368312
C	3.53710679	-3.56478201	-2.00529479
H	3.77247013	-4.35371580	-2.69608239
H	3.67764975	-2.61817646	-2.50704984
H	4.21284530	-3.63466910	-1.16492194
C	1.37148498	-4.84947042	-2.11904182
H	1.05374061	-5.51897072	-1.33255358
H	0.50928920	-4.49509570	-2.66542894
H	2.00090569	-5.39676680	-2.79675177
H	-3.39671756	2.00255851	-0.56626404
N	-2.31688524	4.44501702	-0.70455287
C	-3.56939862	4.33671499	-1.44253929
H	-3.79515485	5.28639840	-1.89787078
H	-3.50264264	3.59583631	-2.23128535
H	-4.39456654	4.07412452	-0.79000867
C	-1.62533595	5.72832608	-0.67130653

H -1.53747037 6.10658556 0.34089208

H -0.63276785 5.65623781 -1.10141078

H -2.18494883 6.44661088 -1.24671989

S1S0-I1

C 1.1265973967 2.0475288856 -1.2053994240

C 0.7855087093 1.0457722175 -0.3738967530

C 0.0326879822 1.2825624088 0.8281850827

C -0.3529586792 2.6319693875 1.1175975820

C -0.0234550462 3.6536564998 0.3035084621

C 0.7458358335 3.4179131285 -0.9076722368

H 1.0706220387 0.0391628318 -0.5988383374

H -0.9198269448 2.8135121148 2.0070072071

H -0.3318251333 4.6462266410 0.5474053372

C -0.2617375764 0.1756732806 1.7783300316

C -1.2410738312 -0.8676640087 1.4231468037

C -2.2166067023 -0.6676030541 0.4423052040

C -1.2430176487 -2.1049754772 2.0997168632

C -3.1681494440 -1.6579038793 0.1552377744

H -2.2748244872 0.2595957500 -0.0975927963

C -2.1792411784 -3.0828930685 1.7887141969

H	-0.5158777928	-2.3009837172	2.8631054327
C	-3.1598872606	-2.8650259098	0.8101363588
H	-3.9088551391	-1.4584972580	-0.5948733059
H	-2.1575034263	-4.0294009387	2.2922834652
N	0.9082221606	-0.0921502985	2.5444598807
H	1.4166349889	-0.9270208722	2.3530052984
H	0.8897924606	0.1517526615	3.5090229801
N	-4.1012208667	-3.9059447349	0.5458628382
C	-4.4762630072	-4.1478739405	-0.8378440886
H	-4.9194574900	-5.1320795771	-0.9171277620
H	-5.1985706792	-3.4272602780	-1.2265410313
H	-3.5963028582	-4.1241209645	-1.4658953737
C	-5.1962625735	-4.0379967408	1.5007934229
H	-4.8170814348	-3.9816388575	2.5111555108
H	-5.9563482886	-3.2640871049	1.3783975971
H	-5.6693604737	-5.0028477952	1.3736142863
H	1.6864141668	1.8358576872	-2.0894712252
N	1.0824516571	4.4053384480	-1.6996276224
C	1.8509755732	4.1740084594	-2.9463182433
H	1.9727330085	5.1115699024	-3.4554858978
H	2.8280339875	3.7756835401	-2.7168312982

H	1.3175926690	3.4983296897	-3.5970267710
C	0.7169499106	5.8090240807	-1.3918072775
H	-0.3562397372	5.9282234738	-1.3974384636
H	1.1184562372	6.1009388282	-0.4335779982
H	1.1373829220	6.4479126580	-2.1455362106

S1S0-I2

C	-2.3134211847	2.5120276130	0.2513674345
C	-1.5366495046	1.9633883089	1.2642048070
C	-0.5324420384	1.0173102759	0.9703412023
C	-0.3480862758	0.6667100813	-0.3722461192
C	-1.1255781689	1.2466516692	-1.3832645017
C	-2.1111220228	2.1590948295	-1.0899466251
H	-1.7072609907	2.2665224201	2.2784491817
H	0.4092240462	-0.0393740364	-0.6587582746
H	-0.9429960618	0.9640427305	-2.4022033365
C	0.3033040218	0.4619734122	2.0460058013
C	1.0842190747	-0.7854883786	1.8294028044
C	0.4308760492	-2.0630112416	1.7547710394
C	2.5151087121	-0.7658625918	1.7693413857
C	1.1266142345	-3.2101429414	1.6424939343

H	-0.6387624976	-2.0838493034	1.7815441502
C	3.2359505203	-1.8985023830	1.6496948837
H	3.0085837012	0.1821480033	1.8259082007
C	2.5779569537	-3.1929387359	1.5888162769
H	0.6071672579	-4.1402974139	1.5734782640
H	4.3018829754	-1.8467045137	1.6205755171
N	-0.0432311266	0.5583308769	3.4232897667
H	0.4038867908	1.2659633868	3.9613734368
H	-0.9907288925	0.3954281415	3.6837517783
N	3.2687238898	-4.3021897455	1.4898344385
C	2.6221696773	-5.6348511790	1.5248000325
H	3.3824532843	-6.3788686182	1.6777857647
H	1.9239430875	-5.6956588099	2.3432740044
H	2.1183829665	-5.8331578969	0.5894350107
C	4.7427082013	-4.3002885121	1.3398496247
H	5.0455674932	-3.6014159990	0.5776363261
H	5.2162252871	-4.0550851446	2.2799521540
H	5.0556793973	-5.2824135668	1.0358320275
H	-3.0901357998	3.2132502127	0.4847837542
N	-2.9314557817	2.7696308075	-2.0871776463
C	-2.5110985888	4.0904004664	-2.5407667206

H	-3.3284471349	4.5672138926	-3.0654845132
H	-2.2512484103	4.7074529274	-1.6924507266
H	-1.6502573779	4.0512560506	-3.2104238040
C	-3.4784452373	1.9154061190	-3.1294905232
H	-2.7566750893	1.6588678302	-3.9069964120
H	-3.8520522741	0.9996231175	-2.6931976200
H	-4.3068168387	2.4237950988	-3.6054424394

S1S0-II

C	-0.023527000	2.517727000	1.042558000
C	-0.971522000	1.623298000	1.411176000
C	-1.886959000	1.063178000	0.484911000
C	-1.789687000	1.475152000	-0.877237000
C	-0.823267000	2.339427000	-1.288285000
C	0.114499000	2.894975000	-0.328023000
H	-1.082764000	1.324548000	2.447831000
H	-2.534001000	1.093223000	-1.566855000
H	-0.773989000	2.629101000	-2.320261000
C	-2.729063000	-0.088448000	0.879717000
C	-1.752760000	-1.169930000	0.625093000
C	-1.510193000	-1.630026000	-0.676012000

C	-0.826984000	-1.545038000	1.641154000
C	-0.429300000	-2.394507000	-0.990144000
H	-2.246863000	-1.379186000	-1.426143000
C	0.239969000	-2.322570000	1.368766000
H	-1.033283000	-1.208030000	2.644961000
C	0.497061000	-2.768682000	0.022241000
H	-0.295899000	-2.735221000	-1.997890000
H	0.889484000	-2.621347000	2.164002000
N	-3.109291000	-0.049085000	2.238656000
H	-3.494045000	-0.873019000	2.588556000
H	-3.599057000	0.739986000	2.527990000
N	1.572715000	-3.531403000	-0.249596000
C	1.812800000	-4.048500000	-1.603246000
H	1.013901000	-4.713186000	-1.918848000
H	1.903199000	-3.244239000	-2.322544000
H	2.736586000	-4.604599000	-1.609675000
C	2.478509000	-3.980230000	0.819481000
H	1.952788000	-4.581558000	1.555095000
H	3.257360000	-4.587581000	0.389670000
H	2.946816000	-3.141808000	1.320703000
H	0.613893000	2.949556000	1.794372000

N	1.071769000	3.743627000	-0.739044000
C	2.042449000	4.330894000	0.203183000
H	2.544682000	3.565551000	0.783748000
H	2.795530000	4.867248000	-0.353605000
H	1.561808000	5.027829000	0.884255000
C	1.177944000	4.169330000	-2.150251000
H	1.421580000	3.335291000	-2.801053000
H	0.257982000	4.627624000	-2.497643000
H	1.964223000	4.902809000	-2.238779000

4.3 Linearly Interpolated Internal Coordinate Paths

S1-I1 to S1S0-I1

Point 1

C	0.00000	0.00000	0.00000
C	1.35539	0.00000	0.00000
C	2.12605	0.00000	1.20767
C	1.41931	-0.00282	2.43700
C	0.04553	-0.01188	2.47125
C	-0.72888	-0.00756	1.23942
H	1.88460	0.01396	-0.93113
H	1.97256	-0.01312	3.35388

H	-0.45827	-0.02394	3.41271
C	3.60284	0.04090	1.14509
C	4.35598	-1.16813	0.81824
C	3.75739	-2.41448	0.75054
C	5.75485	-1.12644	0.59224
C	4.47356	-3.57359	0.45387
H	2.70605	-2.52205	0.93690
C	6.47489	-2.26207	0.29940
H	6.28708	-0.19942	0.67387
C	5.84500	-3.53469	0.21263
H	3.94268	-4.50084	0.42089
H	7.52928	-2.17363	0.14669
N	4.12204	1.31196	0.85773
H	4.93539	1.39899	0.29850
H	3.92839	2.07587	1.46014
N	6.56762	-4.66373	-0.08576
C	5.90332	-5.95543	-0.15394
H	6.62574	-6.71522	-0.40290
H	5.45092	-6.22283	0.79556
H	5.13133	-5.96641	-0.91634
C	8.00277	-4.58707	-0.32023

H	8.23736	-3.94136	-1.15940
H	8.53455	-4.22410	0.55281
H	8.37615	-5.57184	-0.54823
H	-0.52728	0.01726	-0.92791
N	-2.04697	-0.00825	1.27038
C	-2.83734	-0.01152	0.02292
H	-3.88212	-0.03239	0.27263
H	-2.63914	0.88043	-0.55376
H	-2.60853	-0.88614	-0.56816
C	-2.79531	-0.00299	2.54434
H	-2.57887	-0.89235	3.11822
H	-2.55482	0.87557	3.12485
H	-3.84738	0.01286	2.32717

Point 2

C	0.00000	0.00000	0.00000
C	1.35433	0.00000	0.00000
C	2.12351	0.00000	1.20932
C	1.41443	-0.00299	2.43922
C	0.04362	-0.01085	2.47286
C	-0.73006	-0.00599	1.24069

H	1.88452	0.01201	-0.93047
H	1.96821	-0.01300	3.35569
H	-0.46086	-0.02251	3.41392
C	3.60140	0.04594	1.15151
C	4.36014	-1.15756	0.81107
C	3.76985	-2.40987	0.75008
C	5.75420	-1.10160	0.56450
C	4.49504	-3.56200	0.44377
H	2.72202	-2.52711	0.95069
C	6.47979	-2.23231	0.25982
H	6.27738	-0.16857	0.63600
C	5.86032	-3.50814	0.18380
H	3.97445	-4.49576	0.41734
H	7.53092	-2.13781	0.08704
N	4.10532	1.32661	0.86817
H	4.88188	1.42624	0.25988
H	3.96971	2.06440	1.51773
N	6.59669	-4.63258	-0.12618
C	5.92726	-5.91417	-0.28026
H	6.65114	-6.66298	-0.55877
H	5.45279	-6.23535	0.64225

H	5.17216	-5.87408	-1.05786
C	8.04991	-4.56068	-0.19226
H	8.37858	-3.83172	-0.92428
H	8.48642	-4.30466	0.76811
H	8.43845	-5.52219	-0.48685
H	-0.52764	0.01539	-0.92776
N	-2.04723	-0.00499	1.27004
C	-2.83788	-0.00885	0.02198
H	-3.88250	-0.03092	0.27197
H	-2.64052	0.88359	-0.55410
H	-2.60825	-0.88330	-0.56881
C	-2.79709	0.00292	2.54377
H	-2.58470	-0.88782	3.11692
H	-2.55295	0.88022	3.12447
H	-3.84879	0.02362	2.32550

Point 3

C	0.00000	0.00000	0.00000
C	1.35327	0.00000	0.00000
C	2.12096	0.00000	1.21097
C	1.40954	-0.00317	2.44144

C	0.04171	-0.00982	2.47446
C	-0.73125	-0.00441	1.24197
H	1.88444	0.01006	-0.92981
H	1.96386	-0.01288	3.35749
H	-0.46346	-0.02109	3.41512
C	3.59993	0.05098	1.15795
C	4.36432	-1.14677	0.80396
C	3.78278	-2.40512	0.74960
C	5.75312	-1.07626	0.53704
C	4.51710	-3.54999	0.43363
H	2.73876	-2.53225	0.96435
C	6.48436	-2.20182	0.22057
H	6.26676	-0.13720	0.59856
C	5.87581	-3.48094	0.15517
H	4.00720	-4.49029	0.41360
H	7.53181	-2.10105	0.02786
N	4.08840	1.34106	0.87860
H	4.82482	1.45441	0.22364
H	4.01488	2.05121	1.56826
N	6.62607	-4.60038	-0.16657
C	5.95531	-5.86793	-0.40680

H	6.68246	-6.60257	-0.71499
H	5.45996	-6.24265	0.48489
H	5.21730	-5.77663	-1.19583
C	8.07837	-4.54855	-0.06467
H	8.48758	-3.74935	-0.67142
H	8.40919	-4.40578	0.96014
H	8.49192	-5.47884	-0.42085
H	-0.52800	0.01351	-0.92761
N	-2.04749	-0.00172	1.26970
C	-2.83841	-0.00617	0.02104
H	-3.88287	-0.02945	0.27130
H	-2.64189	0.88674	-0.55444
H	-2.60797	-0.88047	-0.56947
C	-2.79888	0.00884	2.54320
H	-2.59053	-0.88326	3.11561
H	-2.55109	0.88485	3.12409
H	-3.85017	0.03438	2.32381

Point 4

C	0.00000	0.00000	0.00000
C	1.35220	0.00000	0.00000

C	2.11842	0.00000	1.21261
C	1.40465	-0.00335	2.44365
C	0.03979	-0.00880	2.47606
C	-0.73244	-0.00283	1.24324
H	1.88436	0.00812	-0.92914
H	1.95951	-0.01275	3.35929
H	-0.46607	-0.01968	3.41633
C	3.59842	0.05602	1.16441
C	4.36852	-1.13576	0.79693
C	3.79618	-2.40023	0.74911
C	5.75162	-1.05042	0.50987
C	4.53974	-3.53756	0.42345
H	2.75626	-2.53747	0.97785
C	6.48858	-2.17064	0.18165
H	6.25522	-0.10532	0.56157
C	5.89146	-3.45310	0.12673
H	4.04093	-4.48439	0.40965
H	7.53193	-2.06338	-0.03082
N	4.07130	1.35529	0.88904
H	4.76433	1.48330	0.19004
H	4.06330	2.03668	1.61131

N	6.65572	-4.56712	-0.20692
C	5.98741	-5.81658	-0.53317
H	6.71961	-6.53384	-0.87080
H	5.47255	-6.24433	0.32383
H	5.26649	-5.67418	-1.32982
C	8.08824	-4.55057	0.05908
H	8.56247	-3.69574	-0.40756
H	8.30576	-4.52488	1.12385
H	8.53580	-5.44257	-0.35132
H	-0.52837	0.01164	-0.92746
N	-2.04774	0.00154	1.26936
C	-2.83893	-0.00350	0.02009
H	-3.88323	-0.02797	0.27063
H	-2.64325	0.88990	-0.55479
H	-2.60768	-0.87763	-0.57013
C	-2.80065	0.01475	2.54262
H	-2.59636	-0.87869	3.11428
H	-2.54923	0.88946	3.12370
H	-3.85152	0.04514	2.32211

Point 5

C	0.00000	0.00000	0.00000
C	1.35114	0.00000	0.00000
C	2.11586	0.00000	1.21426
C	1.39975	-0.00353	2.44585
C	0.03788	-0.00779	2.47766
C	-0.73363	-0.00125	1.24451
H	1.88428	0.00618	-0.92847
H	1.95514	-0.01263	3.36108
H	-0.46867	-0.01828	3.41753
C	3.59687	0.06105	1.17088
C	4.37273	-1.12453	0.78996
C	3.81005	-2.39519	0.74861
C	5.74969	-1.02411	0.48299
C	4.56295	-3.52470	0.41323
H	2.77453	-2.54273	0.99121
C	6.49246	-2.13875	0.14307
H	6.24276	-0.07296	0.52504
C	5.90727	-3.42461	0.09851
H	4.07561	-4.47804	0.40550
H	7.53130	-2.02481	-0.08900

N	4.05400	1.36931	0.89946
H	4.70057	1.51277	0.15933
H	4.11434	2.02120	1.64654
N	6.68563	-4.53279	-0.24722
C	6.02347	-5.76006	-0.65896
H	6.76245	-6.45668	-1.02543
H	5.49064	-6.24000	0.15949
H	5.31944	-5.56688	-1.45946
C	8.07995	-4.56628	0.17559
H	8.60216	-3.67169	-0.13975
H	8.17951	-4.65885	1.25488
H	8.56937	-5.41410	-0.27959
H	-0.52873	0.00977	-0.92730
N	-2.04799	0.00480	1.26901
C	-2.83946	-0.00083	0.01914
H	-3.88359	-0.02649	0.26996
H	-2.64461	0.89305	-0.55514
H	-2.60740	-0.87479	-0.57079
C	-2.80242	0.02067	2.54202
H	-2.60220	-0.87409	3.11294
H	-2.54738	0.89406	3.12332

H	-3.85284	0.05590	2.32040
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Point 6

C	0.00000	0.00000	0.00000
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C	1.35008	0.00000	0.00000
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C	2.11331	0.00000	1.21590
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C	1.39485	-0.00371	2.44805
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C	0.03595	-0.00679	2.47925
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C	-0.73482	0.00033	1.24577
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H	1.88419	0.00424	-0.92779
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H	1.95077	-0.01250	3.36287
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H	-0.47128	-0.01688	3.41873
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C	3.59529	0.06608	1.17737
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C	4.37696	-1.11308	0.78308
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C	3.82438	-2.38998	0.74810
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C	5.74732	-0.99733	0.45642
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C	4.58672	-3.51139	0.40298
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H	2.79356	-2.54803	1.00439
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C	6.49599	-2.10618	0.10487
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H	6.22939	-0.04015	0.48899
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C	5.92323	-3.39547	0.07050
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H	4.11125	-4.47121	0.40113
H	7.52990	-1.98538	-0.14663
N	4.03652	1.38312	0.90988
H	4.63369	1.54262	0.13173
H	4.16731	2.00514	1.67369
N	6.71578	-4.49738	-0.28746
C	6.06336	-5.69828	-0.78376
H	6.81080	-6.37107	-1.17809
H	5.51430	-6.22930	-0.00771
H	5.37584	-5.45489	-1.58436
C	8.05430	-4.59488	0.28155
H	8.60638	-3.67719	0.12481
H	8.03419	-4.80417	1.34963
H	8.59196	-5.39402	-0.20720
H	-0.52909	0.00790	-0.92714
N	-2.04823	0.00806	1.26866
C	-2.83998	0.00185	0.01819
H	-3.88395	-0.02502	0.26929
H	-2.64597	0.89620	-0.55550
H	-2.60711	-0.87196	-0.57146
C	-2.80419	0.02659	2.54142

H	-2.60803	-0.86948	3.11158
H	-2.54553	0.89865	3.12293
H	-3.85413	0.06666	2.31867

Point 7

C	0.00000	0.00000	0.00000
C	1.34902	0.00000	0.00000
C	2.11075	0.00000	1.21754
C	1.38994	-0.00388	2.45024
C	0.03403	-0.00579	2.48085
C	-0.73601	0.00192	1.24704
H	1.88411	0.00231	-0.92711
H	1.94640	-0.01238	3.36465
H	-0.47390	-0.01550	3.41993
C	3.59368	0.07110	1.18387
C	4.38120	-1.10140	0.77627
C	3.83918	-2.38460	0.74756
C	5.74452	-0.97009	0.43017
C	4.61105	-3.49761	0.39269
H	2.81336	-2.55334	1.01741
C	6.49917	-2.07293	0.06703

H	6.21510	-0.00690	0.45345
C	5.93931	-3.36568	0.04271
H	4.14783	-4.46388	0.39655
H	7.52773	-1.94511	-0.20370
N	4.01886	1.39671	0.92029
H	4.56388	1.57267	0.10746
H	4.22149	1.98886	1.69257
N	6.74615	-4.46089	-0.32763
C	6.10697	-5.63120	-0.90717
H	6.86446	-6.27700	-1.32802
H	5.54357	-6.21186	-0.17730
H	5.43539	-5.33843	-1.70420
C	8.01238	-4.63520	0.37385
H	8.57564	-3.71146	0.37895
H	7.87385	-4.95697	1.40533
H	8.60302	-5.38282	-0.13592
H	-0.52945	0.00602	-0.92697
N	-2.04847	0.01132	1.26831
C	-2.84049	0.00452	0.01723
H	-3.88430	-0.02354	0.26861
H	-2.64733	0.89935	-0.55585

H	-2.60682	-0.86912	-0.57213
C	-2.80595	0.03251	2.54081
H	-2.61387	-0.86486	3.11021
H	-2.54369	0.90321	3.12254
H	-3.85539	0.07742	2.31693

Point 8

C	0.00000	0.00000	0.00000
C	1.34795	0.00000	0.00000
C	2.10819	0.00000	1.21918
C	1.38503	-0.00406	2.45243
C	0.03209	-0.00480	2.48244
C	-0.73720	0.00352	1.24830
H	1.88403	0.00038	-0.92642
H	1.94201	-0.01225	3.36642
H	-0.47651	-0.01412	3.42112
C	3.59203	0.07612	1.19039
C	4.38545	-1.08951	0.76954
C	3.85443	-2.37904	0.74701
C	5.74128	-0.94241	0.40425
C	4.63591	-3.48335	0.38236

H	2.83393	-2.55866	1.03025
C	6.50198	-2.03902	0.02959
H	6.19989	0.02674	0.41842
C	5.95552	-3.33524	0.01515
H	4.18533	-4.45602	0.39175
H	7.52480	-1.90401	-0.26020
N	4.00102	1.41007	0.93069
H	4.49136	1.60277	0.08672
H	4.27615	1.97269	1.70307
N	6.77672	-4.42330	-0.36773
C	6.15416	-5.55881	-1.02879
H	6.92316	-6.17454	-1.47444
H	5.57847	-6.18736	-0.34877
H	5.49778	-5.21769	-1.81867
C	7.95558	-4.68575	0.44964
H	8.51125	-3.77291	0.61573
H	7.70269	-5.11308	1.42009
H	8.60214	-5.38078	-0.06772
H	-0.52981	0.00415	-0.92680
N	-2.04871	0.01458	1.26796
C	-2.84101	0.00719	0.01628

H	-3.88465	-0.02206	0.26793
H	-2.64868	0.90250	-0.55621
H	-2.60653	-0.86628	-0.57280
C	-2.80770	0.03843	2.54019
H	-2.61971	-0.86021	3.10882
H	-2.54186	0.90776	3.12215
H	-3.85661	0.08818	2.31518

Point 9

C	0.00000	0.00000	0.00000
C	1.34689	0.00000	0.00000
C	2.10563	0.00000	1.22082
C	1.38011	-0.00424	2.45461
C	0.03016	-0.00381	2.48403
C	-0.73839	0.00511	1.24956
H	1.88394	-0.00155	-0.92572
H	1.93763	-0.01212	3.36819
H	-0.47913	-0.01275	3.42231
C	3.59034	0.08114	1.19692
C	4.38971	-1.07740	0.76290
C	3.87014	-2.37329	0.74643

C	5.73759	-0.91431	0.37867
C	4.66131	-3.46860	0.37199
H	2.85525	-2.56394	1.04291
C	6.50442	-2.00447	-0.00746
H	6.18376	0.06076	0.38392
C	5.97184	-3.30416	-0.01217
H	4.22376	-4.44762	0.38673
H	7.52110	-1.86212	-0.31609
N	3.98299	1.42322	0.94107
H	4.41635	1.63272	0.06968
H	4.33053	1.95696	1.70518
N	6.80746	-4.38461	-0.40772
C	6.20475	-5.48112	-1.14820
H	6.98661	-6.06382	-1.61658
H	5.61900	-6.15548	-0.52160
H	5.56271	-5.09292	-1.92750
C	7.88555	-4.74475	0.50638
H	8.41525	-3.85915	0.82863
H	7.52502	-5.26819	1.39295
H	8.58905	-5.38796	-0.00471
H	-0.53017	0.00228	-0.92663

N	-2.04895	0.01783	1.26760
C	-2.84152	0.00987	0.01532
H	-3.88499	-0.02058	0.26724
H	-2.65003	0.90564	-0.55657
H	-2.60623	-0.86344	-0.57348
C	-2.80945	0.04436	2.53956
H	-2.62556	-0.85555	3.10742
H	-2.54003	0.91229	3.12176
H	-3.85781	0.09894	2.31341

Point 10

C	0.00000	0.00000	0.00000
C	1.34583	0.00000	0.00000
C	2.10306	0.00000	1.22246
C	1.37518	-0.00442	2.45679
C	0.02822	-0.00284	2.48561
C	-0.73959	0.00671	1.25082
H	1.88385	-0.00348	-0.92503
H	1.93323	-0.01199	3.36995
H	-0.48175	-0.01139	3.42350
C	3.58862	0.08615	1.20347

C	4.39398	-1.06507	0.75634
C	3.88630	-2.36733	0.74583
C	5.73346	-0.88579	0.35344
C	4.68723	-3.45335	0.36159
H	2.87734	-2.56919	1.05537
C	6.50649	-1.96928	-0.04409
H	6.16672	0.09512	0.34997
C	5.98827	-3.27242	-0.03924
H	4.26308	-4.43863	0.38149
H	7.51663	-1.81946	-0.37136
N	3.96480	1.43613	0.95144
H	4.33909	1.66236	0.05652
H	4.38386	1.94195	1.69893
N	6.83836	-4.34481	-0.44762
C	6.25859	-5.39816	-1.26503
H	7.05451	-5.94501	-1.75372
H	5.66511	-6.11595	-0.69523
H	5.62985	-4.96438	-2.03045
C	7.80417	-4.81009	0.54191
H	8.29036	-3.96705	1.01167
H	7.34513	-5.41791	1.32389

H	8.56368	-5.40417	0.05084
H	-0.53054	0.00041	-0.92645
N	-2.04918	0.02109	1.26724
C	-2.84202	0.01254	0.01435
H	-3.88533	-0.01909	0.26656
H	-2.65137	0.90879	-0.55694
H	-2.60594	-0.86060	-0.57416
C	-2.81119	0.05029	2.53892
H	-2.63140	-0.85086	3.10600
H	-2.53820	0.91681	3.12136
H	-3.85898	0.10969	2.31163

S1-I2 to S1S0-I2

Point 1

C	0.00000	0.00000	0.00000
C	1.39447	0.00000	0.00000
C	2.13739	0.00000	1.16798
C	1.40551	0.02437	2.38180
C	0.02946	0.02569	2.39738
C	-0.72332	0.00516	1.19045
H	1.88462	0.00831	-0.95460

H	1.92017	0.06987	3.32113
H	-0.47102	0.05302	3.34163
C	3.59873	0.01598	1.16181
C	4.33713	-0.17788	-0.10454
C	4.96088	0.89553	-0.78984
C	4.47531	-1.49008	-0.66252
C	5.66721	0.68812	-1.95024
H	4.86357	1.88764	-0.39856
C	5.17212	-1.72885	-1.80032
H	4.01589	-2.30588	-0.14228
C	5.80569	-0.64892	-2.50729
H	6.11695	1.51822	-2.44917
H	5.25970	-2.72816	-2.16507
N	4.32726	-0.35029	2.30330
H	5.18934	0.09606	2.50721
H	3.86258	-0.76376	3.07465
N	6.48935	-0.85089	-3.61638
C	7.15350	0.25700	-4.33359
H	7.66582	-0.14295	-5.18908
H	6.42732	0.97923	-4.67753
H	7.88027	0.74171	-3.69842

C	6.62393	-2.20435	-4.19151
H	7.14379	-2.85776	-3.50571
H	5.65244	-2.61627	-4.42193
H	7.19189	-2.14123	-5.10135
H	-0.50511	0.00181	-0.94209
N	-2.09648	0.00059	1.21220
C	-2.84347	-0.00942	-0.03528
H	-3.89900	-0.02124	0.18124
H	-2.63483	0.87171	-0.63349
H	-2.61490	-0.88839	-0.62892
C	-2.81967	0.02269	2.47588
H	-2.58443	-0.84173	3.08713
H	-2.60281	0.91838	3.04807
H	-3.87857	0.00676	2.27679

Point 2

C	0.00000000	0.00000000	0.00000000
C	1.39520000	0.00000000	0.00000000
C	2.13579000	0.00000000	1.17151000
C	1.40331000	0.02012000	2.38414000
C	0.02575000	0.01883000	2.39597000

C	-0.72217000	0.00172000	1.18879000
H	1.88709000	0.00984000	-0.95384000
H	1.91761000	0.06127000	3.32389000
H	-0.48070000	0.03937000	3.33759000
C	3.59816000	0.01984000	1.16923000
C	4.34235000	-0.19340000	-0.09176000
C	4.97899000	0.87056000	-0.78318000
C	4.47764000	-1.51257000	-0.63505000
C	5.69372000	0.64876000	-1.93226000
H	4.88405000	1.86624000	-0.40071000
C	5.18354000	-1.76529000	-1.76299000
H	4.00632000	-2.31998000	-0.11257000
C	5.83094000	-0.69442000	-2.47450000
H	6.15451000	1.47118000	-2.43378000
H	5.26624000	-2.76780000	-2.12008000
N	4.33054000	-0.33911000	2.31339000
H	5.15124000	0.16522000	2.55171000
H	3.87540000	-0.79969000	3.06421000
N	6.52431000	-0.91189000	-3.57354000
C	7.19270000	0.18605000	-4.30295000
H	7.68829000	-0.22306000	-5.16398000

H	6.47094000	0.91545000	-4.63999000
H	7.93318000	0.66353000	-3.67808000
C	6.66864000	-2.27335000	-4.12847000
H	7.15848000	-2.92254000	-3.41755000
H	5.70261000	-2.68000000	-4.38951000
H	7.27042000	-2.22432000	-5.01722000
H	-0.50643000	0.00347000	-0.94189000
N	-2.10139000	-0.00314000	1.21324000
C	-2.84478000	-0.11900000	-0.03108000
H	-3.90036000	-0.14911000	0.18599000
H	-2.66336000	0.72478000	-0.69017000
H	-2.58686000	-1.02931000	-0.56125000
C	-2.81188000	0.21579000	2.46559000
H	-2.22323644	0.83966627	3.10525957
H	-3.74851552	0.69287925	2.26559060
H	-2.98587598	-0.72433044	2.94600540

Point 3

C	0.00000000	0.00000000	0.00000000
C	1.39593000	0.00000000	0.00000000
C	2.13417000	0.00000000	1.17503000

C	1.40110000	0.01587000	2.38647000
C	0.02206000	0.01197000	2.39453000
C	-0.72101000	-0.00171000	1.18712000
H	1.88956000	0.01136000	-0.95308000
H	1.91505000	0.05269000	3.32661000
H	-0.49033000	0.02574000	3.33346000
C	3.59755000	0.02370000	1.17665000
C	4.34762000	-0.20886000	-0.07859000
C	4.99724000	0.84555000	-0.77581000
C	4.48004000	-1.53480000	-0.60713000
C	5.72041000	0.60951000	-1.91322000
H	4.90463000	1.84472000	-0.40216000
C	5.19506000	-1.80135000	-1.72487000
H	3.99683000	-2.33376000	-0.08273000
C	5.85635000	-0.73963000	-2.44058000
H	6.19225000	1.42419000	-2.41702000
H	5.27298000	-2.80695000	-2.07433000
N	4.33375000	-0.32788000	2.32348000
H	5.10799000	0.22972000	2.59736000
H	3.89134000	-0.83456000	3.05265000
N	6.55946000	-0.97247000	-3.52918000

C	7.23227000	0.11529000	-4.27061000
H	7.71108000	-0.30291000	-5.13679000
H	6.51535000	0.85199000	-4.60102000
H	7.98618000	0.58517000	-3.65598000
C	6.71343000	-2.34165000	-4.06359000
H	7.17256000	-2.98599000	-3.32866000
H	5.75424000	-2.74381000	-4.35532000
H	7.34827000	-2.30635000	-4.92975000
H	-0.50774000	0.00512000	-0.94169000
N	-2.10629000	-0.00689000	1.21430000
C	-2.84585000	-0.22833000	-0.01798000
H	-3.90036000	-0.27690000	0.20349000
H	-2.69230000	0.57297000	-0.73569000
H	-2.55863000	-1.16446000	-0.48326000
C	-2.80476000	0.40550000	2.42423000
H	-2.20911708	1.11905580	2.95427493
H	-3.74244715	0.84875924	2.16123942
H	-2.97578212	-0.44839089	3.04593876

Point 4

C	0.00000000	0.00000000	0.00000000
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C	1.39667000	0.00000000	0.00000000
C	2.13254000	0.00000000	1.17856000
C	1.39889000	0.01164000	2.38878000
C	0.01838000	0.00513000	2.39307000
C	-0.71986000	-0.00513000	1.18544000
H	1.89204000	0.01289000	-0.95230000
H	1.91250000	0.04414000	3.32929000
H	-0.49990000	0.01213000	3.32923000
C	3.59691000	0.02757000	1.18408000
C	4.35294000	-0.22423000	-0.06502000
C	5.01562000	0.82051000	-0.76769000
C	4.48249000	-1.55676000	-0.57876000
C	5.74726000	0.57038000	-1.89311000
H	4.92529000	1.82308000	-0.40290000
C	5.20669000	-1.83702000	-1.68597000
H	3.98741000	-2.34723000	-0.05277000
C	5.88192000	-0.78450000	-2.40551000
H	6.23015000	1.37727000	-2.39891000
H	5.27991000	-2.84560000	-2.02785000
N	4.33687000	-0.31660000	2.33355000
H	5.05996000	0.28910000	2.64392000

H	3.91032000	-0.86815000	3.04003000
N	6.59476000	-1.03259000	-3.48329000
C	7.27218000	0.04474000	-4.23656000
H	7.73417000	-0.38243000	-5.10754000
H	6.56053000	0.78888000	-4.56063000
H	8.03923000	0.50664000	-3.63209000
C	6.75827000	-2.40921000	-3.99686000
H	7.18603000	-3.04811000	-3.23910000
H	5.80731000	-2.80767000	-4.31930000
H	7.42535000	-2.38724000	-4.83894000
H	-0.50906000	0.00677000	-0.94149000
N	-2.11119000	-0.01064000	1.21537000
C	-2.84662000	-0.33666000	0.00398000
H	-3.89890000	-0.40332000	0.23371000
H	-2.72152000	0.41714000	-0.76958000
H	-2.53023000	-1.29304000	-0.39551000
C	-2.79844000	0.58692000	2.35255000
H	-2.19634574	1.37142186	2.76113211
H	-3.73702753	0.98801682	2.03149736
H	-2.96688663	-0.15981018	3.10020440

Point 5

C	0.00000000	0.00000000	0.00000000
C	1.39740000	0.00000000	0.00000000
C	2.13089000	0.00000000	1.18207000
C	1.39668000	0.00742000	2.39108000
C	0.01471000	-0.00171000	2.39159000
C	-0.71870000	-0.00854000	1.18375000
H	1.89450000	0.01440000	-0.95153000
H	1.90996000	0.03562000	3.33194000
H	-0.50942000	-0.00146000	3.32490000
C	3.59623000	0.03144000	1.19152000
C	4.35831000	-0.23951000	-0.05106000
C	5.03414000	0.79547000	-0.75884000
C	4.48499000	-1.57846000	-0.54995000
C	5.77425000	0.53139000	-1.87191000
H	4.94603000	1.80134000	-0.40292000
C	5.21842000	-1.87229000	-1.64628000
H	3.97807000	-2.36039000	-0.02271000
C	5.90762000	-0.82904000	-2.36930000
H	6.26820000	1.33044000	-2.37942000
H	5.28702000	-2.88374000	-1.98063000

N	4.33992000	-0.30527000	2.34360000
H	5.00759000	0.34297000	2.69111000
H	3.93228000	-0.90026000	3.02642000
N	6.63019000	-1.09224000	-3.43588000
C	7.31240000	-0.02557000	-4.20081000
H	7.75755000	-0.46159000	-5.07620000
H	6.60645000	0.72612000	-4.51879000
H	8.09231000	0.42797000	-3.60640000
C	6.80313000	-2.47600000	-3.92830000
H	7.19891000	-3.10890000	-3.14891000
H	5.86180000	-2.87155000	-4.28137000
H	7.50158000	-2.46692000	-4.74484000
H	-0.51038000	0.00842000	-0.94128000
N	-2.11609000	-0.01439000	1.21646000
C	-2.84705000	-0.44325000	0.03471000
H	-3.89591000	-0.52711000	0.27649000
H	-2.75092000	0.25819000	-0.79144000
H	-2.50162000	-1.41431000	-0.29863000
C	-2.79303000	0.75531000	2.25211000
H	-2.18507461	1.59065275	2.53048517
H	-3.73237694	1.10644665	1.87897413

H -2.95872578 0.13403300 3.10736423

Point 6

C 0.00000000 0.00000000 0.00000000

C 1.39813000 0.00000000 0.00000000

C 2.12923000 0.00000000 1.18559000

C 1.39448000 0.00322000 2.39337000

C 0.01106000 -0.00853000 2.39009000

C -0.71755000 -0.01194000 1.18205000

H 1.89697000 0.01592000 -0.95074000

H 1.90743000 0.02712000 3.33455000

H -0.51889000 -0.01503000 3.32049000

C 3.59552000 0.03533000 1.19897000

C 4.36373000 -0.25470000 -0.03670000

C 5.05277000 0.77043000 -0.74924000

C 4.48754000 -1.59987000 -0.52070000

C 5.80137000 0.49256000 -1.84963000

H 4.96683000 1.77951000 -0.40221000

C 5.23022000 -1.90715000 -1.60581000

H 3.96880000 -2.37325000 0.00746000

C 5.93343000 -0.87321000 -2.33195000

H	6.30637000	1.28374000	-2.35854000
H	5.29430000	-2.92136000	-1.93269000
N	4.34289000	-0.29390000	2.35364000
H	4.95131000	0.39094000	2.73868000
H	3.95715000	-0.93069000	3.01187000
N	6.66574000	-1.15138000	-3.38694000
C	7.35293000	-0.09560000	-4.16333000
H	7.78121000	-0.54034000	-5.04279000
H	6.65309000	0.66375000	-4.47551000
H	8.14540000	0.34920000	-3.57888000
C	6.84798000	-2.54198000	-3.85791000
H	7.21122000	-3.16837000	-3.05812000
H	5.91766000	-2.93539000	-4.24147000
H	7.57686000	-2.54530000	-4.64749000
H	-0.51170000	0.01007000	-0.94106000
N	-2.12098000	-0.01816000	1.21755000
C	-2.84708000	-0.54734000	0.07404000
H	-3.89134000	-0.64702000	0.33156000
H	-2.78040000	0.09705000	-0.80093000
H	-2.47283000	-1.52759000	-0.19329000
C	-2.78863000	0.90619000	2.12519000

H	-2.17544025	1.77138001	2.26782441
H	-3.72860704	1.20022885	1.70699827
H	-2.95202365	0.42560825	3.06712614

Point 7

C	0.00000000	0.00000000	0.00000000
C	1.39886000	0.00000000	0.00000000
C	2.12756000	0.00000000	1.18910000
C	1.39227000	-0.00097000	2.39565000
C	0.00743000	-0.01534000	2.38857000
C	-0.71639000	-0.01534000	1.18034000
H	1.89944000	0.01744000	-0.94996000
H	1.90490000	0.01865000	3.33712000
H	-0.52831000	-0.02858000	3.31597000
C	3.59477000	0.03921000	1.20642000
C	4.36918000	-0.26979000	-0.02194000
C	5.07151000	0.74540000	-0.73888000
C	4.49014000	-1.62099000	-0.49101000
C	5.82860000	0.45392000	-1.82626000
H	4.98770000	1.75761000	-0.40077000
C	5.24209000	-1.94157000	-1.56457000

H	3.95961000	-2.38579000	0.03772000
C	5.95935000	-0.91699000	-2.29345000
H	6.34465000	1.23718000	-2.33627000
H	5.30175000	-2.95844000	-1.88402000
N	4.34578000	-0.28248000	2.36367000
H	4.89163000	0.43272000	2.78636000
H	3.98483000	-0.95922000	2.99647000
N	6.70138000	-1.20999000	-3.33647000
C	7.39373000	-0.16534000	-4.12413000
H	7.80514000	-0.61863000	-5.00730000
H	6.70043000	0.60177000	-4.43077000
H	8.19846000	0.27035000	-3.54949000
C	6.89279000	-2.60712000	-3.78568000
H	7.22296000	-3.22650000	-2.96678000
H	5.97488000	-2.99918000	-4.19953000
H	7.65112000	-2.62230000	-4.54692000
H	-0.51302000	0.01172000	-0.94085000
N	-2.12587000	-0.02193000	1.21865000
C	-2.84669000	-0.64821000	0.12176000
H	-3.88512000	-0.76182000	0.39851000
H	-2.80985000	-0.06528000	-0.79780000

H	-2.44385000	-1.63228000	-0.08022000
C	-2.78528000	1.03551000	1.97476000
H	-2.16748701	1.90912935	1.97934805
H	-3.72577295	1.26614246	1.51958786
H	-2.94662998	0.70748810	2.98037813

Point 8

C	0.00000000	0.00000000	0.00000000
C	1.39960000	0.00000000	0.00000000
C	2.12587000	0.00000000	1.19260000
C	1.39006000	-0.00515000	2.39792000
C	0.00381000	-0.02214000	2.38703000
C	-0.71524000	-0.01872000	1.17862000
H	1.90191000	0.01895000	-0.94916000
H	1.90238000	0.01021000	3.33966000
H	-0.53767000	-0.04210000	3.31137000
C	3.59399000	0.04311000	1.21388000
C	4.37466000	-0.28477000	-0.00680000
C	5.09035000	0.72041000	-0.72777000
C	4.49277000	-1.64183000	-0.46090000
C	5.85593000	0.41547000	-1.80179000

H	5.00861000	1.73565000	-0.39858000
C	5.25402000	-1.97556000	-1.52256000
H	3.95049000	-2.39803000	0.06807000
C	5.98536000	-0.96036000	-2.25381000
H	6.38300000	1.19080000	-2.31259000
H	5.30935000	-2.99498000	-1.83464000
N	4.34860000	-0.27101000	2.37368000
H	4.82907000	0.46802000	2.83389000
H	4.01521000	-0.98568000	2.98027000
N	6.73709000	-1.26803000	-3.28448000
C	7.43478000	-0.23474000	-4.08319000
H	7.82932000	-0.69642000	-4.96975000
H	6.74842000	0.54022000	-4.38457000
H	8.25147000	0.19145000	-3.51822000
C	6.93753000	-2.67138000	-3.71162000
H	7.23416000	-3.28332000	-2.87492000
H	6.03340000	-3.06285000	-4.15548000
H	7.72428000	-2.69784000	-4.44318000
H	-0.51434000	0.01337000	-0.94062000
N	-2.13075000	-0.02571000	1.21977000
C	-2.84582000	-0.74516000	0.17759000

H	-3.87721000	-0.87033000	0.47682000
H	-2.83915000	-0.22779000	-0.78187000
H	-2.41471000	-1.72784000	0.03981000
C	-2.78296000	1.13971000	1.80444000
H	-2.16117127	2.00035475	1.67189041
H	-3.72387130	1.30166288	1.32136941
H	-2.94252129	0.97246224	2.84917364

Point 9

C	0.00000000	0.00000000	0.00000000
C	1.40033000	0.00000000	0.00000000
C	2.12417000	0.00000000	1.19610000
C	1.38785000	-0.00932000	2.40018000
C	0.00020000	-0.02894000	2.38547000
C	-0.71409000	-0.02209000	1.17689000
H	1.90437000	0.02046000	-0.94836000
H	1.89987000	0.00180000	3.34217000
H	-0.54698000	-0.05561000	3.30667000
C	3.59317000	0.04701000	1.22135000
C	4.38018000	-0.29963000	0.00874000
C	5.10929000	0.69546000	-0.71590000

C	4.49543000	-1.66236000	-0.43036000
C	5.88334000	0.37725000	-1.77622000
H	5.02957000	1.71364000	-0.39565000
C	5.26600000	-2.00908000	-1.47978000
H	3.94145000	-2.40997000	0.09850000
C	6.01143000	-1.00331000	-2.21302000
H	6.42142000	1.14462000	-2.28751000
H	5.31709000	-3.03096000	-1.78455000
N	4.35133000	-0.25950000	2.38368000
H	4.76416000	0.49664000	2.88100000
H	4.04817000	-1.00987000	2.96335000
N	6.77283000	-1.32547000	-3.23096000
C	7.47606000	-0.30377000	-4.04050000
H	7.85373000	-0.77368000	-4.93012000
H	6.79706000	0.47910000	-4.33691000
H	8.30439000	0.11253000	-3.48505000
C	6.98216000	-2.73472000	-3.63574000
H	7.24483000	-3.33882000	-2.78257000
H	6.09320000	-3.12637000	-4.10925000
H	7.79624000	-2.77184000	-4.33633000
H	-0.51565000	0.01502000	-0.94039000

N	-2.13562000	-0.02950000	1.22090000
C	-2.84446000	-0.83750000	0.24116000
H	-3.86756000	-0.97141000	0.56584000
H	-2.86821000	-0.38943000	-0.75304000
H	-2.38541000	-1.81381000	0.16601000
C	-2.78165000	1.21582000	1.61837000
H	-2.15644711	2.04254573	1.35276519
H	-3.72289673	1.30505298	1.11737892
H	-2.93967192	1.21369434	2.67663488

Point 10

C	0.00000	0.00000	0.00000
C	1.40106	0.00000	0.00000
C	2.12246	0.00000	1.19960
C	1.38564	-0.01347	2.40242
C	-0.00339	-0.03572	2.38388
C	-0.71294	-0.02545	1.17515
H	1.90683	0.02196	-0.94756
H	1.89737	-0.00658	3.34464
H	-0.55623	-0.06909	3.30189
C	3.59232	0.05091	1.22882

C	4.38573	-0.31438	0.02468
C	5.12830	0.67057	-0.70326
C	4.49812	-1.68259	-0.39940
C	5.91082	0.33927	-1.74956
H	5.05056	1.69159	-0.39197
C	5.27801	-2.04214	-1.43625
H	3.93249	-2.42160	0.12900
C	6.03755	-1.04581	-2.17110
H	6.45988	1.09867	-2.26100
H	5.32497	-3.06638	-1.73375
N	4.35399	-0.24794	2.39366
H	4.69748	0.51842	2.92742
H	4.08357	-1.03163	2.94578
N	6.80860	-1.38230	-3.17591
C	7.51754	-0.37241	-3.99607
H	7.87837	-0.85034	-4.88844
H	6.84631	0.41845	-4.28776
H	8.35720	0.03363	-3.44995
C	7.02667	-2.79711	-3.55804
H	7.25499	-3.39302	-2.68978
H	6.15423	-3.18970	-4.06078

H	7.86694	-2.84423	-4.22642
H	-0.51697	0.01667	-0.94016
N	-2.14049	-0.03330	1.22203
C	-2.84258	-0.92459	0.31209
H	-3.85615	-1.06401	0.66482
H	-2.89691	-0.54913	-0.71131
H	-2.35600	-1.88979	0.29755
C	-2.78124	1.26157	1.42111
H	-3.81081	1.11128	1.71796
H	-2.28030	1.80479	2.20971
H	-2.77056	1.87928	0.52148

S1-II to S1S0-II

Point 1

C	0.00000	0.00000	0.00000
C	1.37593	0.00000	0.00000
C	2.11239	0.00000	1.19188
C	1.39064	-0.01607	2.39087
C	0.01529	-0.02040	2.41063
C	-0.72875	-0.01156	1.21032
H	1.89563	0.00660	-0.93861

H	1.91782	-0.00031	3.32555
H	-0.48552	-0.01375	3.35464
C	3.59776	-0.01565	1.18873
C	4.16353	-1.34483	1.52713
C	4.50304	-1.70259	2.85918
C	4.31967	-2.33519	0.51849
C	4.97378	-2.95407	3.17525
H	4.39887	-0.97300	3.63657
C	4.80503	-3.59132	0.80483
H	4.06739	-2.08602	-0.49192
C	5.14297	-3.95809	2.15417
H	5.22626	-3.17921	4.18813
H	4.93412	-4.29645	0.01315
N	4.24459	0.68089	0.16326
H	5.23680	0.65916	0.12387
H	3.83614	1.53383	-0.14245
N	5.59550	-5.16700	2.44708
C	5.94117	-5.54215	3.83109
H	6.73808	-4.91771	4.20892
H	5.07813	-5.46038	4.47605
H	6.27643	-6.56317	3.84117

C	5.77156	-6.19270	1.40184
H	6.48333	-5.86263	0.65876
H	6.14764	-7.09123	1.85595
H	4.82818	-6.41935	0.92620
H	-0.51349	0.01244	-0.93730
N	-2.09446	-0.01125	1.21873
C	-2.84280	0.01436	-0.03249
H	-2.63108	-0.85812	-0.64021
H	-3.89747	0.01838	0.18627
H	-2.61836	0.90273	-0.61195
C	-2.82645	-0.01485	2.47941
H	-2.59792	-0.89580	3.06864
H	-2.60319	0.86531	3.07196
H	-3.88393	-0.01801	2.27465

Point 2

C	0.00000	0.00000	0.00000
C	1.37354	0.00000	0.00000
C	2.11244	0.00000	1.19253
C	1.39183	-0.01376	2.39572
C	0.01824	-0.02228	2.41716

C	-0.72646	-0.02031	1.21513
H	1.89741	0.00933	-0.93775
H	1.92557	0.00756	3.32796
H	-0.48329	-0.01599	3.36133
C	3.59670	-0.04220	1.18339
C	4.10027	-1.40437	1.48457
C	4.38687	-1.82224	2.80925
C	4.22030	-2.36920	0.44624
C	4.77268	-3.10770	3.09629
H	4.31136	-1.10686	3.60445
C	4.62126	-3.65810	0.70037
H	4.00825	-2.06857	-0.56034
C	4.90293	-4.08583	2.04275
H	4.98872	-3.37789	4.10707
H	4.72822	-4.34375	-0.11166
N	4.24129	0.63409	0.14107
H	5.22940	0.58041	0.08557
H	3.86023	1.50397	-0.14395
N	5.27556	-5.33067	2.30784
C	5.57060	-5.76512	3.68547
H	6.39838	-5.20358	4.09598

H	4.70305	-5.64672	4.31902
H	5.84027	-6.80577	3.67223
C	5.42228	-6.33067	1.23412
H	6.17318	-6.02004	0.52092
H	5.73297	-7.26411	1.66742
H	4.48194	-6.48761	0.72484
H	-0.51495	0.01664	-0.93736
N	-2.08972	-0.02539	1.22185
C	-2.84032	-0.00851	-0.03032
H	-2.61416	-0.87531	-0.64093
H	-3.89494	-0.02391	0.18934
H	-2.63143	0.88580	-0.60696
C	-2.82731	-0.02367	2.48185
H	-2.60384	-0.90408	3.07409
H	-2.60362	0.85750	3.07288
H	-3.88421	-0.02363	2.27305

Point 3

C	0.00000	0.00000	0.00000
C	1.37116	0.00000	0.00000
C	2.11250	0.00000	1.19319

C	1.39305	-0.01144	2.40056
C	0.02122	-0.02414	2.42371
C	-0.72413	-0.02905	1.22000
H	1.89920	0.01207	-0.93686
H	1.93332	0.01545	3.33029
H	-0.48101	-0.01824	3.36806
C	3.59514	-0.06881	1.17835
C	4.03478	-1.46013	1.44144
C	4.26548	-1.93406	2.75585
C	4.11967	-2.39736	0.37437
C	4.56404	-3.24750	3.01145
H	4.21885	-1.23481	3.56886
C	4.43426	-3.71282	0.59453
H	3.95091	-2.04881	-0.62587
C	4.65659	-4.19658	1.92706
H	4.74135	-3.56015	4.01802
H	4.51982	-4.37798	-0.23705
N	4.23702	0.58716	0.11949
H	5.21975	0.50140	0.04834
H	3.88533	1.47285	-0.14573
N	4.94670	-5.47168	2.16240

C	5.18827	-5.96132	3.53117
H	6.04302	-5.46596	3.97210
H	4.31935	-5.80474	4.15491
H	5.39069	-7.01692	3.49337
C	5.06492	-6.44499	1.06154
H	5.85290	-6.15874	0.37788
H	5.30803	-7.40850	1.47228
H	4.13225	-6.53113	0.52155
H	-0.51642	0.02085	-0.93739
N	-2.08492	-0.03954	1.22506
C	-2.83774	-0.03141	-0.02801
H	-2.59732	-0.89226	-0.64155
H	-3.89194	-0.06623	0.19259
H	-2.64457	0.86859	-0.60178
C	-2.82812	-0.03257	2.48433
H	-2.60971	-0.91245	3.07952
H	-2.60405	0.84957	3.07388
H	-3.88440	-0.02939	2.27146

Point 4

C	0.00000	0.00000	0.00000
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C	1.36877	0.00000	0.00000
C	2.11256	0.00000	1.19384
C	1.39428	-0.00912	2.40540
C	0.02424	-0.02600	2.43027
C	-0.72175	-0.03779	1.22491
H	1.90099	0.01479	-0.93595
H	1.94108	0.02336	3.33255
H	-0.47867	-0.02050	3.37481
C	3.59309	-0.09546	1.17362
C	3.96726	-1.51196	1.39785
C	4.13931	-2.03758	2.69922
C	4.01812	-2.41959	0.30299
C	4.34874	-3.37266	2.92121
H	4.12161	-1.35651	3.53002
C	4.24478	-3.75513	0.48766
H	3.89544	-2.02695	-0.68854
C	4.40505	-4.28967	1.80770
H	4.48518	-3.72491	3.92155
H	4.30969	-4.39883	-0.36266
N	4.23178	0.54013	0.09856
H	5.20783	0.42219	0.01221

H	3.91135	1.44039	-0.14783
N	4.61040	-5.58905	2.01159
C	4.79593	-6.12950	3.36919
H	5.67348	-5.70325	3.83816
H	3.92888	-5.93353	3.98477
H	4.92978	-7.19515	3.30572
C	4.70097	-6.53474	0.88487
H	5.52363	-6.27761	0.23017
H	4.87464	-7.52324	1.27145
H	3.78066	-6.54947	0.31711
H	-0.51788	0.02505	-0.93741
N	-2.08004	-0.05369	1.22837
C	-2.83507	-0.05432	-0.02556
H	-2.58055	-0.90897	-0.64206
H	-3.88849	-0.10858	0.19602
H	-2.65777	0.85109	-0.59643
C	-2.82889	-0.04156	2.48684
H	-2.61551	-0.92091	3.08492
H	-2.60448	0.84153	3.07498
H	-3.88452	-0.03529	2.26986

Point 5

C	0.00000	0.00000	0.00000
C	1.36639	0.00000	0.00000
C	2.11263	0.00000	1.19449
C	1.39554	-0.00679	2.41024
C	0.02730	-0.02784	2.43685
C	-0.71932	-0.04653	1.22988
H	1.90278	0.01751	-0.93501
H	1.94884	0.03130	3.33472
H	-0.47627	-0.02278	3.38159
C	3.59053	-0.12215	1.16918
C	3.89791	-1.55972	1.35390
C	4.00886	-2.13240	2.63965
C	3.91597	-2.43580	0.23224
C	4.12774	-3.48245	2.82607
H	4.01995	-1.47162	3.48816
C	4.05359	-3.78473	0.38014
H	3.84188	-2.00321	-0.74838
C	4.14946	-4.36453	1.68529
H	4.22135	-3.87124	3.81827
H	4.09866	-4.40606	-0.48810

N	4.22558	0.49304	0.07826
H	5.19364	0.34288	-0.02280
H	3.93819	1.40648	-0.15030
N	4.26822	-5.68193	1.85620
C	4.39545	-6.26858	3.20053
H	5.29142	-5.91403	3.69506
H	3.53360	-6.03238	3.80970
H	4.45975	-7.33917	3.11048
C	4.33200	-6.59911	0.70489
H	5.18658	-6.37563	0.07836
H	4.43471	-7.60730	1.06592
H	3.42876	-6.54233	0.11233
H	-0.51935	0.02926	-0.93740
N	-2.07509	-0.06785	1.23176
C	-2.83230	-0.07726	-0.02296
H	-2.56386	-0.92542	-0.64247
H	-3.88457	-0.15094	0.19963
H	-2.67102	0.83330	-0.59089
C	-2.82960	-0.05064	2.48939
H	-2.62124	-0.92946	3.09030
H	-2.60491	0.83337	3.07617

H	-3.88456	-0.04132	2.26826
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Point 6

C	0.00000	0.00000	0.00000
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C	1.36400	0.00000	0.00000
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C	2.11269	0.00000	1.19513
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C	1.39681	-0.00445	2.41506
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C	0.03039	-0.02968	2.44345
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C	-0.71684	-0.05527	1.23490
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H	1.90457	0.02023	-0.93405
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H	1.95659	0.03926	3.33682
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H	-0.47382	-0.02508	3.38839
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C	3.58748	-0.14886	1.16505
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C	3.82696	-1.60331	1.30969
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C	3.87466	-2.21812	2.57741
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C	3.81355	-2.44594	0.16227
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C	3.90206	-3.57625	2.72654
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H	3.91421	-1.57987	3.44350
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C	3.86150	-3.80141	0.27235
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H	3.79027	-1.97781	-0.80544
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C	3.89103	-4.42074	1.56044
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H	3.95107	-3.99830	3.70882
H	3.88756	-4.39950	-0.61301
N	4.21842	0.44590	0.05860
H	5.17719	0.26355	-0.05666
H	3.96575	1.37105	-0.15315
N	3.92182	-5.74964	1.69711
C	3.98877	-6.37768	3.02625
H	4.89859	-6.09700	3.54375
H	3.13551	-6.10076	3.63079
H	3.98292	-7.44794	2.90886
C	3.95966	-6.63748	0.52241
H	4.84304	-6.45188	-0.07696
H	3.99027	-7.65984	0.85669
H	3.07817	-6.50955	-0.09197
H	-0.52081	0.03346	-0.93738
N	-2.07007	-0.08202	1.23525
C	-2.82944	-0.10022	-0.02022
H	-2.54726	-0.94164	-0.64278
H	-3.88019	-0.19331	0.20342
H	-2.68433	0.81523	-0.58517
C	-2.83027	-0.05981	2.49197

H	-2.62691	-0.93811	3.09564
H	-2.60534	0.82509	3.07745
H	-3.88451	-0.04748	2.26667

Point 7

C	0.00000	0.00000	0.00000
C	1.36162	0.00000	0.00000
C	2.11276	0.00000	1.19577
C	1.39811	-0.00211	2.41988
C	0.03353	-0.03150	2.45007
C	-0.71432	-0.06400	1.23997
H	1.90636	0.02294	-0.93306
H	1.96435	0.04724	3.33884
H	-0.47132	-0.02738	3.39522
C	3.58393	-0.17557	1.16122
C	3.75464	-1.64261	1.26533
C	3.73726	-2.29443	2.51281
C	3.71122	-2.44998	0.09320
C	3.67278	-3.65353	2.62318
H	3.80474	-1.68100	3.39627
C	3.66933	-3.80503	0.16468

H	3.74060	-1.95094	-0.85976
C	3.63102	-4.45795	1.43382
H	3.67563	-4.10540	3.59385
H	3.67726	-4.37905	-0.73699
N	4.21031	0.39875	0.03960
H	5.15848	0.18428	-0.08935
H	3.99390	1.33402	-0.15641
N	3.57289	-5.79163	1.53517
C	3.57793	-6.45611	2.84740
H	4.49684	-6.25107	3.38522
H	2.73668	-6.13834	3.44914
H	3.50170	-7.52062	2.70212
C	3.58565	-6.64935	0.33827
H	4.49440	-6.50555	-0.23514
H	3.54339	-7.68024	0.64481
H	2.73054	-6.45112	-0.29499
H	-0.52228	0.03767	-0.93733
N	-2.06497	-0.09620	1.23883
C	-2.82648	-0.12320	-0.01734
H	-2.53074	-0.95762	-0.64300
H	-3.87535	-0.23569	0.20739

H	-2.69768	0.79686	-0.57926
C	-2.83088	-0.06907	2.49460
H	-2.63252	-0.94684	3.10096
H	-2.60576	0.81670	3.07882
H	-3.88438	-0.05379	2.26509

Point 8

C	0.00000	0.00000	0.00000
C	1.35924	0.00000	0.00000
C	2.11283	0.00000	1.19640
C	1.39943	0.00025	2.42470
C	0.03670	-0.03331	2.45670
C	-0.71174	-0.07272	1.24508
H	1.90815	0.02564	-0.93204
H	1.97211	0.05524	3.34077
H	-0.46876	-0.02970	3.40208
C	3.57989	-0.20228	1.15771
C	3.68119	-1.67754	1.22094
C	3.59725	-2.36106	2.44615
C	3.60930	-2.44790	0.02518
C	3.44101	-3.71387	2.51653

H	3.69189	-1.77478	3.34669
C	3.47790	-3.79552	0.05752
H	3.69287	-1.92278	-0.91142
C	3.37069	-4.47597	1.30605
H	3.39638	-4.19196	3.47405
H	3.46862	-4.34467	-0.85968
N	4.20124	0.35162	0.02124
H	5.13751	0.10516	-0.12083
H	4.02254	1.29532	-0.16011
N	3.22318	-5.80755	1.37126
C	3.16502	-6.50336	2.66507
H	4.08813	-6.37532	3.22046
H	2.33920	-6.14503	3.26584
H	3.01858	-7.55665	2.49154
C	3.21170	-6.63439	0.15330
H	4.14211	-6.53597	-0.39555
H	3.09623	-7.66804	0.43131
H	2.38752	-6.36717	-0.49593
H	-0.52375	0.04188	-0.93726
N	-2.05980	-0.11037	1.24251
C	-2.82343	-0.14619	-0.01433

H	-2.51432	-0.97335	-0.64311
H	-3.87004	-0.27805	0.21152
H	-2.71106	0.77820	-0.57316
C	-2.83144	-0.07842	2.49726
H	-2.63806	-0.95567	3.10626
H	-2.60618	0.80819	3.08028
H	-3.88417	-0.06022	2.26351

Point 9

C	0.00000	0.00000	0.00000
C	1.35685	0.00000	0.00000
C	2.11290	0.00000	1.19703
C	1.40078	0.00261	2.42951
C	0.03990	-0.03511	2.46335
C	-0.70911	-0.08144	1.25025
H	1.90994	0.02834	-0.93100
H	1.97986	0.06326	3.34263
H	-0.46615	-0.03203	3.40896
C	3.57534	-0.22897	1.15450
C	3.60684	-1.70804	1.17660
C	3.45523	-2.41777	2.37772

C	3.50816	-2.43974	-0.04167
C	3.20790	-3.75696	2.40717
H	3.57605	-1.86102	3.29500
C	3.28807	-3.77288	-0.04875
H	3.64707	-1.89351	-0.96048
C	3.11134	-4.47472	1.17779
H	3.11469	-4.25752	3.35012
H	3.26251	-4.29640	-0.98068
N	4.19123	0.30454	0.00355
H	5.11431	0.02627	-0.15110
H	4.05152	1.25487	-0.16427
N	2.87448	-5.79720	1.20627
C	2.75216	-6.51917	2.48034
H	3.67449	-6.46904	3.05053
H	1.94517	-6.12091	3.08200
H	2.53609	-7.55568	2.27840
C	2.83961	-6.59241	-0.03165
H	3.78768	-6.54258	-0.55750
H	2.65098	-7.62300	0.21726
H	2.05076	-6.25798	-0.69400
H	-0.52522	0.04609	-0.93717

N	-2.05456	-0.12455	1.24627
C	-2.82028	-0.16920	-0.01117
H	-2.49799	-0.98885	-0.64314
H	-3.86427	-0.32039	0.21583
H	-2.72448	0.75926	-0.56688
C	-2.83195	-0.08786	2.49996
H	-2.64353	-0.96459	3.11152
H	-2.60660	0.79957	3.08183
H	-3.88388	-0.06680	2.26194

Point 10

C	0.00000	0.00000	0.00000
C	1.35447	0.00000	0.00000
C	2.11298	0.00000	1.19766
C	1.40214	0.00497	2.43431
C	0.04315	-0.03690	2.47002
C	-0.70644	-0.09015	1.25546
H	1.91174	0.03103	-0.92993
H	1.98762	0.07131	3.34440
H	-0.46348	-0.03437	3.41587
C	3.57031	-0.25564	1.15161

C	3.53186	-1.73406	1.13243
C	3.31181	-2.46442	2.30783
C	3.40813	-2.42552	-0.10722
C	2.97463	-3.78260	2.29567
H	3.45762	-1.93955	3.24140
C	3.10068	-3.73718	-0.15374
H	3.60316	-1.86328	-1.00701
C	2.85426	-4.45422	1.04968
H	2.83200	-4.30180	3.22277
H	3.05981	-4.23436	-1.09961
N	4.18027	0.25754	-0.01348
H	5.08888	-0.05230	-0.18011
H	4.08074	1.21262	-0.16889
N	2.52857	-5.76056	1.04109
C	2.34151	-6.50345	2.29430
H	3.25800	-6.53170	2.87646
H	1.55667	-6.06628	2.89871
H	2.05681	-7.51763	2.06399
C	2.47117	-6.52342	-0.21573
H	3.43269	-6.52496	-0.72029
H	2.20985	-7.54508	0.00372

H	1.72188	-6.12398	-0.88841
H	-0.52669	0.05029	-0.93706
N	-2.04924	-0.13874	1.25012
C	-2.81703	-0.19222	-0.00787
H	-2.48177	-1.00411	-0.64307
H	-3.85804	-0.36271	0.22030
H	-2.73792	0.74001	-0.56040
C	-2.83241	-0.09738	2.50269
H	-2.64893	-0.97361	3.11676
H	-2.60700	0.79083	3.08347
H	-3.88350	-0.07351	2.26038