

Supporting Information: QM/MM Studies on Excited-State Relaxation Mechanism of a Semisynthetic dTPT3 Base

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1. Active Orbitals in CASSCF and MS-CASPT2 Computations

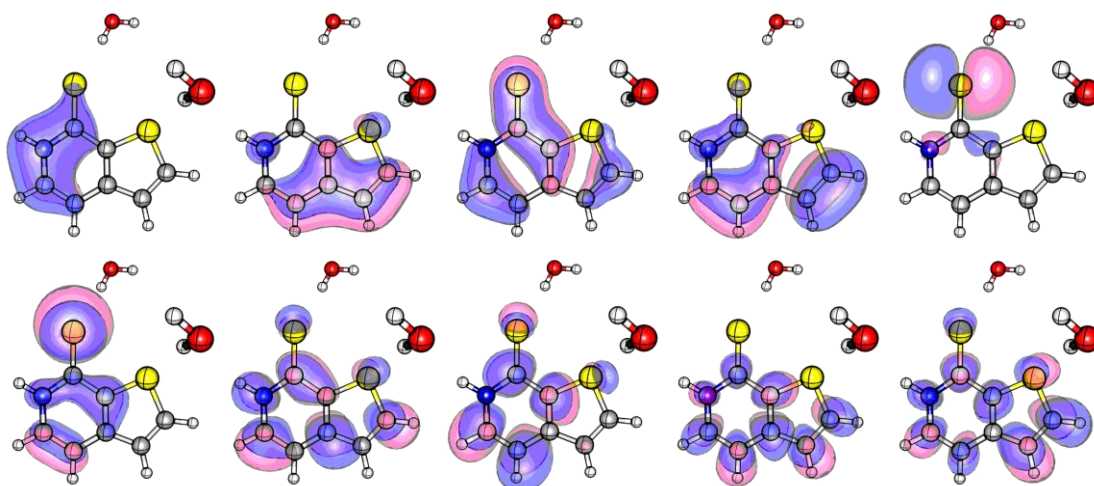


Fig. S1: Molecular orbitals used for the active space of CASSCF and MS-CASPT2 calculations.

2. Spin-Orbit Couplings

Spin-orbit coupling matrix elements are calculated with the atomic mean-field approximation, based on which the effective spin-orbit coupling $\langle \Psi_I | H_{eff}^{SO} | \Psi_J \rangle$ is calculated

$$\langle \Psi_I | H_{eff}^{SO} | \Psi_J \rangle = \sqrt{\frac{(\langle \Psi_I | H_x^{SO} | \Psi_J \rangle)^2 + (\langle \Psi_I | H_y^{SO} | \Psi_J \rangle)^2 + (\langle \Psi_I | H_z^{SO} | \Psi_J \rangle)^2}{3}}$$

in which Ψ_I and Ψ_J are electronic wavefunctions of involved two electronic states and H_x^{SO} , H_y^{SO} , H_z^{SO} are x, y, and z components of the spin-orbit operator.

3. Crossing Point and Conical Intersection

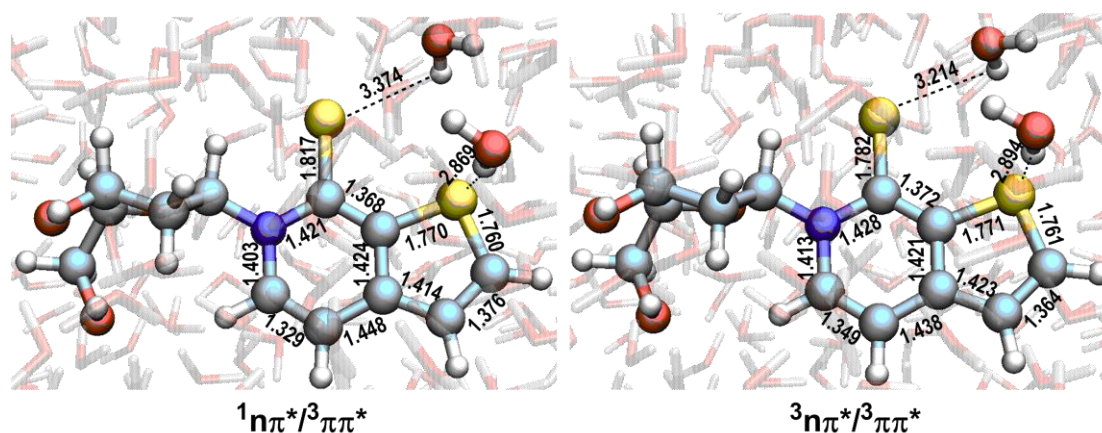


Fig. S2: Optimized structures of minimum-energy crossing point and conical intersection. Also shown are selected bond lengths (in Å) optimized at the QM(CASSCF)/MM level.

4. Linearly Interpolated Cartesian Coordinate Paths

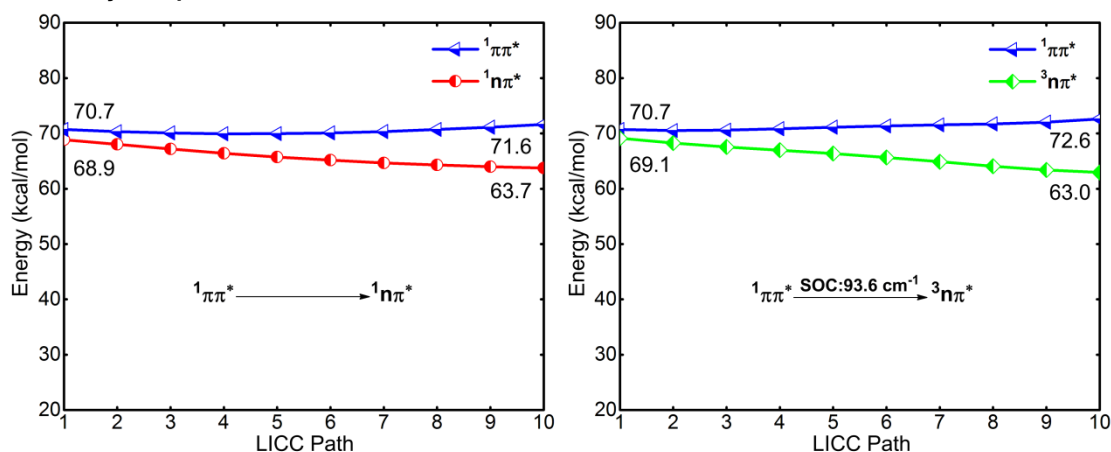


Fig. S3: QM(MS-CASPT2)/MM computed linearly interpolated Cartesian coordinate paths (LICCs, in kcal/mol) connecting (left) the $S_2(1\pi\pi^*)$ and $S_1(1n\pi^*)$ minima and (right) the $S_2(1\pi\pi^*)$ and $T_2(3n\pi^*)$ minima.

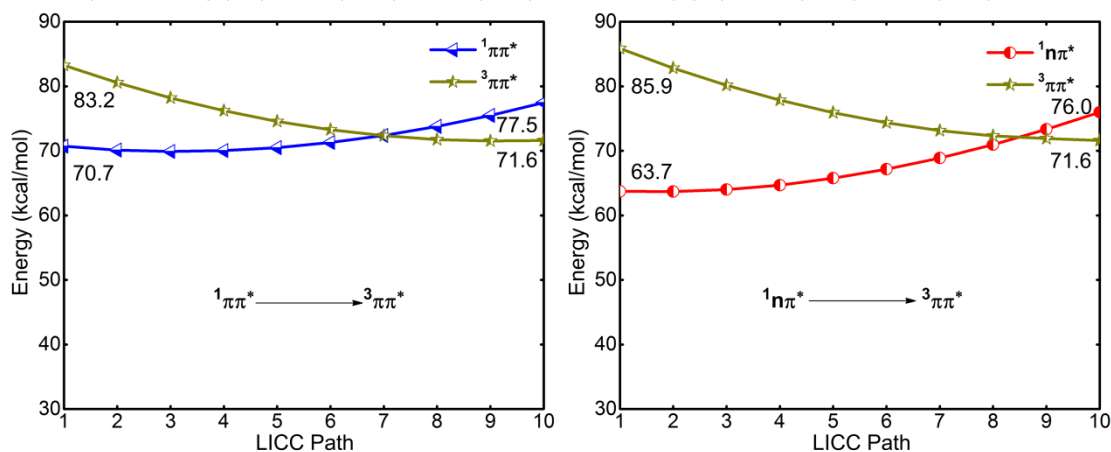


Fig. S4: QM(MS-CASPT2)/MM computed linearly interpolated Cartesian coordinate paths (LICCs, in kcal/mol) connecting (left) the $S_2(1\pi\pi^*)$ and $T_3(3\pi\pi^*)$ minimum and (right) the $S_1(1n\pi^*)$ and $T_3(3\pi\pi^*)$ minima.

5. Vertical Excitation Energies

Table S1: Vertical Excitation Energies (in kcal/mol) of dTPT3 to the Lowest $S_1(1n\pi^*)$, $S_2(1\pi\pi^*)$, $T_1(3\pi\pi^*)$, $T_2(3n\pi^*)$, and $T_3(3\pi\pi^*)$ Electronic States at the Franck-Condon Point Computed by QM(MS-CASPT2)/MM. (snapshot taken from 10 ps MD, QM includes dTPT3 and 2 water molecules)

States	$S_1(1n\pi^*)$	$S_2(1\pi\pi^*)$	$T_1(3\pi\pi^*)$	$T_2(3n\pi^*)$	$T_3(3\pi\pi^*)$
Energies	72.6	77.5	61.9	71.5	78.2

Table S2: Vertical Excitation Energies (in kcal/mol) of dTPT3 to the Lowest $S_1(1n\pi^*)$, $S_2(1\pi\pi^*)$, $T_1(3\pi\pi^*)$, $T_2(3n\pi^*)$, and $T_3(3\pi\pi^*)$ Electronic States at the Franck-Condon Point Computed by QM(MS-CASPT2)/MM. (snapshot taken from 1 ns MD, QM includes dTPT3 and 2 water molecules)

States	$S_1(1n\pi^*)$	$S_2(1\pi\pi^*)$	$T_1(3\pi\pi^*)$	$T_2(3n\pi^*)$	$T_3(3\pi\pi^*)$
Energies	74.3	78.5	63.1	73.3	79.4

Table S3: Vertical Excitation Energies (in kcal/mol) of dTPT3 to the Lowest $S_1(1n\pi^*)$, $S_2(1\pi\pi^*)$, $T_1(3\pi\pi^*)$, $T_2(3n\pi^*)$, and $T_3(3\pi\pi^*)$ Electronic States at the Franck-Condon Point Computed by QM(MS-CASPT2)/MM.

(snapshot taken from 10 ps MD, QM includes dTPT3 and 8 water molecules)

States	S ₁ (1nπ*)	S ₂ (1ππ*)	T ₁ (3ππ*)	T ₂ (3nπ*)	T ₃ (3ππ*)
Energies	75.0	79.3	62.6	74.0	78.7

Table S4: Vertical Excitation Energies (in kcal/mol) of dTPT3 to the Lowest S₁ (1nπ*), S₂ (1ππ*), T₁ (3ππ*), T₂ (3nπ*), and T₃ (3ππ*) Electronic States at the Franck-Condon Point Computed by QM(MS-CASPT2)/MM. (MD=10ps, QM includes dTPT3)

States	S ₁ (1nπ*)	S ₂ (1ππ*)	T ₁ (3ππ*)	T ₂ (3nπ*)	T ₃ (3ππ*)
Energies	71.0	77.6	61.1	69.7	77.5

Table S5: Vertical Excitation Energies (in kcal/mol) to the Lowest S₁ (1nπ*), S₂ (1ππ*), T₁ (3ππ*), T₂ (3nπ*), and T₃ (3ππ*) Electronic States of (a) the dTPT3 Chromophore and (b) the dTPT3 Chromophore with the nearby sugar moiety Computed by MS-CASPT2.

States		S ₁ (1nπ*)	S ₂ (1ππ*)	T ₁ (3ππ*)	T ₂ (3nπ*)	T ₃ (3ππ*)
Energies	a	72.2	77.2	61.4	71.0	76.1
	b	73.1	78.2	63.4	72.0	79.3

6. Cartesian Coordinates of All Optimized Structures and Paths

In xyz format (unit: Ångstrom)

S ₀			
C	3.145563000	-1.017282000	0.058384000
C	3.139450000	0.356708000	-0.021779000
C	1.938702000	1.154406000	-0.215838000
C	0.782422000	-0.986993000	-0.234175000
C	1.905077000	-1.719106000	-0.065368000
C	4.471654000	-1.557305000	0.256867000
C	5.410507000	-0.586601000	0.320078000
N	0.777901000	0.396611000	-0.270028000
H	-0.172380000	-1.458993000	-0.347630000
H	1.852453000	-2.789563000	-0.039071000
H	4.680108000	-2.605327000	0.348939000
H	6.464082000	-0.711313000	0.464723000
S	1.989479000	2.797819000	-0.337968000
S	4.746603000	1.017168000	0.131138000
C	-0.545674000	1.042047000	-0.205315000
O	-1.352431000	0.687636000	-1.335241000
C	-1.353978000	0.667782000	1.017081000
H	-0.468837000	2.128676000	-0.226833000
C	-2.726721000	0.726103000	-0.923906000
C	-2.730508000	1.043112000	0.563027000
H	-1.038291000	1.202769000	1.916920000

H	-1.318606000	-0.402232000	1.239579000
H	-3.209952000	1.546053000	-1.459930000
H	-2.864286000	2.119549000	0.699434000
C	-3.416005000	-0.574432000	-1.329515000
H	-4.486323000	-0.526567000	-1.114767000
H	-3.284121000	-0.757703000	-2.399194000
O	-2.878415000	-1.696570000	-0.640282000
H	-2.841215000	-1.449991000	0.299332000
O	-3.749242000	0.370637000	1.293211000
H	-3.542180000	0.495192000	2.234734000
O	3.852240000	5.681236000	-1.945592000
H	3.391549000	4.865908000	-1.794074000
H	4.718602000	5.544189000	-1.586657000
O	4.769933000	2.214144000	3.641807000
H	4.830324000	2.075327000	2.705636000
H	3.995453000	2.747996000	3.762198000
S _i (1nπ*)			
C	3.168010000	-1.042290000	0.103688000
C	3.135126000	0.388565000	0.008919000
C	1.982508000	1.093285000	-0.186874000
C	0.785599000	-1.006763000	-0.250452000
C	1.918243000	-1.722202000	-0.065151000
C	4.475253000	-1.549645000	0.295311000
C	5.440759000	-0.575928000	0.351958000
N	0.757405000	0.394479000	-0.244975000
H	-0.159306000	-1.487760000	-0.400968000
H	1.866131000	-2.794467000	-0.069424000
H	4.699533000	-2.594860000	0.388321000
H	6.493231000	-0.700630000	0.494209000
S	2.016687000	2.860941000	-0.371244000
S	4.774635000	1.045681000	0.166021000
C	-0.545491000	1.062583000	-0.145435000
O	-1.356002000	0.768778000	-1.289194000
C	-1.355847000	0.643970000	1.059857000
H	-0.438018000	2.146365000	-0.116825000
C	-2.729345000	0.776633000	-0.873476000
C	-2.730019000	1.046432000	0.621926000
H	-1.035300000	1.136864000	1.981846000
H	-1.325305000	-0.434989000	1.234662000
H	-3.225279000	1.605742000	-1.383562000
H	-2.854292000	2.119206000	0.792237000
C	-3.403957000	-0.520232000	-1.315883000

H	-4.475673000	-0.487387000	-1.105270000
H	-3.265736000	-0.675123000	-2.389169000
O	-2.860547000	-1.655932000	-0.653993000
H	-2.833340000	-1.435895000	0.292534000
O	-3.753940000	0.359569000	1.330707000
H	-3.556521000	0.470104000	2.276088000
O	3.738932000	5.560076000	-1.919442000
H	3.522233000	4.773061000	-2.406992000
H	4.630856000	5.434899000	-1.624613000
O	4.875584000	2.229662000	3.692186000
H	4.916938000	1.827126000	2.834401000
H	4.044706000	2.684184000	3.711689000
S ₂ (¹ ΠΠ*)			
C	3.141221000	-1.102899000	0.079226000
C	3.117087000	0.365888000	-0.017711000
C	1.972624000	1.063409000	-0.190414000
C	0.761152000	-1.000704000	-0.230371000
C	1.928584000	-1.747254000	-0.042164000
C	4.464016000	-1.594669000	0.273491000
C	5.402277000	-0.607660000	0.324689000
N	0.764092000	0.371463000	-0.270608000
H	-0.186630000	-1.483157000	-0.345625000
H	1.846139000	-2.817142000	-0.007927000
H	4.705340000	-2.635066000	0.373157000
H	6.455612000	-0.739690000	0.463629000
S	1.921829000	2.841912000	-0.340868000
S	4.760960000	1.031858000	0.131335000
C	-0.551513000	1.034594000	-0.199561000
O	-1.360926000	0.692345000	-1.330905000
C	-1.362116000	0.663215000	1.022064000
H	-0.473911000	2.119295000	-0.214456000
C	-2.734369000	0.731112000	-0.918676000
C	-2.736609000	1.046493000	0.568478000
H	-1.043691000	1.195412000	1.922735000
H	-1.331855000	-0.407022000	1.242887000
H	-3.217855000	1.551266000	-1.454074000
H	-2.865151000	2.123513000	0.706674000
C	-3.422414000	-0.569525000	-1.325484000
H	-4.492744000	-0.521771000	-1.111586000
H	-3.289662000	-0.752532000	-2.395162000
O	-2.885376000	-1.691974000	-0.636374000
H	-2.840290000	-1.442459000	0.302166000

O	-3.757788000	0.377100000	1.297797000
H	-3.547760000	0.496965000	2.239246000
O	3.847065000	5.683179000	-1.940925000
H	3.408607000	4.850621000	-1.830882000
H	4.710638000	5.555861000	-1.572410000
O	4.817912000	2.198328000	3.645998000
H	4.890663000	1.982088000	2.724811000
H	4.036436000	2.729113000	3.714868000
T ₁ (³ ππ*)			
C	3.136559000	-1.045431000	0.179610000
C	3.100809000	0.395915000	0.001487000
C	1.934976000	1.087828000	-0.203328000
C	0.750615000	-1.016208000	-0.145227000
C	1.899246000	-1.724372000	0.038217000
C	4.451238000	-1.535224000	0.372502000
C	5.406823000	-0.556467000	0.357314000
N	0.708511000	0.383147000	-0.111892000
H	-0.191401000	-1.507989000	-0.275652000
H	1.852642000	-2.797027000	0.057372000
H	4.682816000	-2.573366000	0.514926000
H	6.462581000	-0.673575000	0.484568000
S	1.951023000	2.794331000	-0.554554000
S	4.740024000	1.058793000	0.085006000
C	-0.586961000	1.055185000	0.022140000
O	-1.383232000	0.848584000	-1.150614000
C	-1.419219000	0.573576000	1.188634000
H	-0.459774000	2.132354000	0.129312000
C	-2.761850000	0.824235000	-0.753351000
C	-2.782364000	1.013795000	0.753746000
H	-1.110390000	1.012163000	2.141611000
H	-1.400677000	-0.513244000	1.305246000
H	-3.259232000	1.674706000	-1.225892000
H	-2.897727000	2.077222000	0.979984000
C	-3.422255000	-0.452463000	-1.271088000
H	-4.496506000	-0.436621000	-1.072223000
H	-3.270593000	-0.550217000	-2.349178000
O	-2.881388000	-1.618378000	-0.661825000
H	-2.859540000	-1.444046000	0.294348000
O	-3.823316000	0.299853000	1.408633000
H	-3.629658000	0.340299000	2.360260000
O	3.755298000	5.597983000	-1.872912000
H	4.084950000	4.716041000	-1.976523000

H	4.075824000	5.883208000	-1.028468000
O	4.943279000	2.289250000	3.619960000
H	4.935550000	1.924303000	2.744622000
H	4.128292000	2.764887000	3.698612000
T ₂ (³ nπ*)			
C	3.156471000	-1.046750000	0.153865000
C	3.134334000	0.371931000	0.025260000
C	1.980005000	1.082367000	-0.181744000
C	0.777179000	-1.008731000	-0.225075000
C	1.906925000	-1.728472000	-0.038877000
C	4.469536000	-1.557346000	0.349476000
C	5.433404000	-0.591214000	0.371320000
N	0.746420000	0.391170000	-0.155900000
H	-0.168150000	-1.483811000	-0.389513000
H	1.857175000	-2.800640000	-0.063653000
H	4.692161000	-2.600921000	0.464933000
H	6.486637000	-0.715908000	0.508755000
S	2.012389000	2.825155000	-0.525371000
S	4.772619000	1.027245000	0.148301000
C	-0.542797000	1.068818000	0.007986000
O	-1.363435000	0.877362000	-1.150781000
C	-1.352963000	0.571578000	1.182665000
H	-0.409444000	2.144937000	0.125324000
C	-2.734362000	0.856813000	-0.726662000
C	-2.722951000	1.022533000	0.783396000
H	-1.022834000	0.991710000	2.136559000
H	-1.335667000	-0.517425000	1.277874000
H	-3.234149000	1.718559000	-1.175409000
H	-2.830215000	2.082332000	1.029488000
C	-3.416889000	-0.405708000	-1.250804000
H	-4.485944000	-0.386671000	-1.024774000
H	-3.293410000	-0.484603000	-2.334032000
O	-2.868886000	-1.586135000	-0.676934000
H	-2.825603000	-1.431037000	0.281765000
O	-3.751334000	0.300610000	1.448845000
H	-3.530161000	0.315301000	2.395298000
O	3.680747000	5.540776000	-1.749229000
H	3.565457000	4.896719000	-2.434574000
H	4.600388000	5.510892000	-1.524142000
O	4.894056000	2.244604000	3.705794000
H	4.942331000	1.885598000	2.829392000
H	4.063591000	2.699164000	3.740387000

T₃(³ππ*)

C	3.169551000	-1.043074000	0.062706000
C	3.160334000	0.342746000	-0.018246000
C	1.927992000	1.122911000	-0.212200000
C	0.748004000	-0.971834000	-0.236676000
C	1.954734000	-1.750376000	-0.049776000
C	4.505029000	-1.564287000	0.261463000
C	5.439074000	-0.587613000	0.323076000
N	0.772076000	0.385471000	-0.271884000
H	-0.201523000	-1.448892000	-0.348774000
H	1.892959000	-2.818335000	-0.015601000
H	4.725482000	-2.609681000	0.356426000
H	6.493489000	-0.705310000	0.465882000
S	1.983567000	2.818080000	-0.340589000
S	4.764655000	1.014831000	0.135823000
C	-0.545684000	1.047995000	-0.203482000
O	-1.357066000	0.708988000	-1.335983000
C	-1.357752000	0.678684000	1.018974000
H	-0.460332000	2.134041000	-0.219387000
C	-2.730696000	0.737439000	-0.921973000
C	-2.734360000	1.053373000	0.564742000
H	-1.042142000	1.215372000	1.917918000
H	-1.324224000	-0.390133000	1.245955000
H	-3.220526000	1.554217000	-1.456740000
H	-2.869088000	2.129446000	0.702734000
C	-3.413025000	-0.566927000	-1.328699000
H	-4.483663000	-0.524429000	-1.114800000
H	-3.279981000	-0.749261000	-2.398401000
O	-2.872029000	-1.687514000	-0.639816000
H	-2.841905000	-1.443981000	0.300818000
O	-3.752050000	0.378337000	1.294044000
H	-3.541850000	0.497135000	2.235598000
O	3.848674000	5.683332000	-1.944371000
H	3.392877000	4.862869000	-1.816333000
H	4.712110000	5.545635000	-1.579576000
O	4.793069000	2.211304000	3.656855000
H	4.857548000	2.043092000	2.725969000
H	4.013669000	2.739415000	3.761519000

¹ππ*/³ππ*

C	3.210278000	-0.806598000	0.153924000
C	3.070894000	0.596091000	-0.047913000
C	1.855670000	1.203640000	-0.205448000

C	0.826085000	-0.967823000	-0.048052000
C	1.992513000	-1.588244000	0.095858000
C	4.557995000	-1.211175000	0.293731000
C	5.456988000	-0.173488000	0.206722000
N	0.675406000	0.426718000	-0.055263000
H	-0.088465000	-1.520735000	-0.134430000
H	2.022714000	-2.659775000	0.143311000
H	4.858769000	-2.229416000	0.453182000
H	6.523090000	-0.215699000	0.285763000
S	1.727553000	2.983659000	-0.546101000
S	4.660299000	1.374107000	-0.051639000
C	-0.653112000	1.021080000	0.095129000
O	-1.438853000	0.794298000	-1.078719000
C	-1.457654000	0.477932000	1.253529000
H	-0.582895000	2.100734000	0.221778000
C	-2.814926000	0.725898000	-0.678074000
C	-2.835607000	0.883459000	0.833480000
H	-1.159129000	0.900743000	2.216755000
H	-1.403308000	-0.610232000	1.339261000
H	-3.336140000	1.572745000	-1.130687000
H	-2.982157000	1.937809000	1.082795000
C	-3.439566000	-0.557779000	-1.220035000
H	-4.512460000	-0.579281000	-1.014341000
H	-3.292142000	-0.626271000	-2.301069000
O	-2.857024000	-1.719215000	-0.640824000
H	-2.837059000	-1.567123000	0.319242000
O	-3.850222000	0.124667000	1.478374000
H	-3.650727000	0.149011000	2.429408000
O	4.143232000	5.085254000	-1.376010000
H	4.303127000	4.504646000	-2.108160000
H	4.847661000	4.916429000	-0.764338000
O	4.949071000	1.927731000	3.709254000
H	4.922894000	1.723046000	2.783659000
H	4.136824000	2.382982000	3.884173000

${}^3\pi\pi^*/{}^3\pi\pi\pi^*$

C	3.221740000	-0.808990000	0.204430000
C	3.113421000	0.587094000	-0.038355000
C	1.906813000	1.211761000	-0.226081000
C	0.830162000	-0.938956000	-0.027452000
C	2.007273000	-1.576937000	0.139797000
C	4.569815000	-1.241635000	0.349764000
C	5.480716000	-0.233284000	0.232963000

N	0.705520000	0.468764000	-0.013726000
H	-0.091794000	-1.475311000	-0.126363000
H	2.028600000	-2.649344000	0.181429000
H	4.847698000	-2.262269000	0.531686000
H	6.545793000	-0.296667000	0.311845000
S	1.766319000	2.947419000	-0.604695000
S	4.722332000	1.327494000	-0.068464000
C	-0.608287000	1.089436000	0.159376000
O	-1.398754000	0.918012000	-1.021238000
C	-1.423850000	0.530180000	1.302531000
H	-0.511207000	2.162202000	0.322662000
C	-2.775156000	0.845536000	-0.623356000
C	-2.795919000	0.964284000	0.891388000
H	-1.121529000	0.926898000	2.275858000
H	-1.383630000	-0.560095000	1.364226000
H	-3.291707000	1.705832000	-1.055573000
H	-2.930720000	2.013612000	1.167662000
C	-3.405352000	-0.421058000	-1.198545000
H	-4.478987000	-0.441126000	-0.996703000
H	-3.254967000	-0.463751000	-2.280472000
O	-2.832308000	-1.600333000	-0.646499000
H	-2.812528000	-1.471213000	0.316828000
O	-3.820590000	0.200772000	1.514288000
H	-3.622924000	0.198681000	2.466089000
O	4.047072000	4.798968000	-1.092271000
H	4.295291000	4.425815000	-1.928017000
H	4.834616000	4.784013000	-0.562816000
O	4.914974000	2.011749000	3.697272000
H	4.934318000	1.745086000	2.787228000
H	4.064827000	2.413207000	3.816626000

FC point to S₂(¹ππ*) minimum

coord_1

C	3.145563900	-1.017282300	0.058384000
C	3.139450900	0.356708100	-0.021779000
C	1.938702500	1.154406300	-0.215838100
C	0.782422200	-0.986993300	-0.234175100
C	1.905077500	-1.719106500	-0.065368000
C	4.471655300	-1.557305400	0.256867100
C	5.410508500	-0.586601200	0.320078100
N	0.777901200	0.396611100	-0.270028100
H	-0.172380000	-1.458993400	-0.347630100
H	1.852453500	-2.789563800	-0.039071000

H	4.680109300	-2.605327700	0.348939100
H	6.464083800	-0.711313200	0.464723100
S	1.989479600	2.797819800	-0.337968100
S	4.746604300	1.017168300	0.131138000
C	-0.545674200	1.042047300	-0.205315100
O	-1.352431400	0.687636200	-1.335241400
C	-1.353978400	0.667782200	1.017081300
H	-0.468837100	2.128676600	-0.226833100
C	-2.726721800	0.726103200	-0.923906300
C	-2.730508800	1.043112300	0.563027200
H	-1.038291300	1.202769300	1.916920500
H	-1.318606400	-0.402232100	1.239579300
H	-3.209952900	1.546053400	-1.459930400
H	-2.864286800	2.119549600	0.699434200
C	-3.416006000	-0.574432200	-1.329515400
H	-4.486324300	-0.526567100	-1.114767300
H	-3.284121900	-0.757703200	-2.399194700
O	-2.878415800	-1.696570500	-0.640282200
H	-2.841215800	-1.449991400	0.299332100
O	-3.749243000	0.370637100	1.293211400
H	-3.542181000	0.495192100	2.234734600
O	3.852241100	5.681237600	-1.945592500
H	3.391549900	4.865909400	-1.794074500
H	4.718603300	5.544190600	-1.586657400
O	4.769934300	2.214144600	3.641808000
H	4.830325400	2.075327600	2.705636800
H	3.995454100	2.747996800	3.762199100
coord_2			
C	3.145078700	-1.026781700	0.060690500
C	3.136963100	0.357741600	-0.021337300
C	1.942468600	1.144308800	-0.213024000
C	0.780056100	-0.988503700	-0.233761900
C	1.907686800	-1.722220700	-0.062798700
C	4.470803900	-1.561443000	0.258705300
C	5.409591200	-0.588926900	0.320580900
N	0.776363900	0.393829900	-0.270102900
H	-0.173966000	-1.461665500	-0.347416500
H	1.851749500	-2.792614800	-0.035618700
H	4.682910400	-2.608618000	0.351621800
H	6.463139900	-0.714451800	0.464592100
S	1.981959500	2.802732100	-0.338302400
S	4.748196500	1.018814400	0.131149200

C	-0.546326000	1.041232000	-0.204686600
O	-1.353378200	0.688171300	-1.334770300
C	-1.354885700	0.667288300	1.017624300
H	-0.469404100	2.127647100	-0.225469500
C	-2.727574500	0.726671700	-0.923335900
C	-2.731189700	1.043501000	0.563621800
H	-1.038894500	1.201966100	1.917555600
H	-1.320081400	-0.402750600	1.239937000
H	-3.210834100	1.546644200	-1.459291100
H	-2.864386200	2.120003100	0.700226900
C	-3.416720800	-0.573875300	-1.329077400
H	-4.487040500	-0.526022700	-1.114423800
H	-3.284740300	-0.757117800	-2.398756400
O	-2.879191900	-1.696047700	-0.639857100
H	-2.841115700	-1.449141700	0.299637700
O	-3.750195600	0.371368600	1.293710300
H	-3.542804100	0.495403200	2.235225300
O	3.851662300	5.681465800	-1.945088000
H	3.393441700	4.864223100	-1.798177700
H	4.717714700	5.545500100	-1.585088300
O	4.775262000	2.212403600	3.642262100
H	4.837026400	2.064983400	2.707755900
H	4.000004300	2.745914900	3.756928200
coord_3			
C	3.144593500	-1.036281100	0.062997000
C	3.134475400	0.358775200	-0.020895700
C	1.946234600	1.134211200	-0.210210000
C	0.777690100	-0.990014100	-0.233348600
C	1.910296000	-1.725334900	-0.060229400
C	4.469952600	-1.565580600	0.260543500
C	5.408674000	-0.591252700	0.321083600
N	0.774826600	0.391048600	-0.270177800
H	-0.175552000	-1.464337600	-0.347202800
H	1.851045500	-2.795665800	-0.032166400
H	4.685711400	-2.611908300	0.354304500
H	6.462196000	-0.717590400	0.464461100
S	1.974439500	2.807644500	-0.338636700
S	4.749788600	1.020460500	0.131160300
C	-0.546977800	1.040416700	-0.204058200
O	-1.354325100	0.688706500	-1.334299200
C	-1.355792900	0.666794400	1.018167200
H	-0.469971200	2.126617600	-0.224106000

C	-2.728427300	0.727240300	-0.922765600
C	-2.731870700	1.043889700	0.564216500
H	-1.039497600	1.201162900	1.918190700
H	-1.321556400	-0.403269100	1.240294600
H	-3.211715300	1.547234900	-1.458651800
H	-2.864485600	2.120456700	0.701019600
C	-3.417435700	-0.573318500	-1.328639400
H	-4.487756700	-0.525478200	-1.114080400
H	-3.285358700	-0.756532400	-2.398318200
O	-2.879967900	-1.695524800	-0.639431900
H	-2.841015600	-1.448292000	0.299943300
O	-3.751148200	0.372100100	1.294209300
H	-3.543427100	0.495614300	2.235716000
O	3.851083600	5.681694000	-1.944583500
H	3.395333400	4.862536900	-1.802281000
H	4.716826100	5.546809700	-1.583519200
O	4.780589600	2.210662700	3.642716300
H	4.843727400	2.054639300	2.709875100
H	4.004554500	2.743833100	3.751657400
coord_4			
C	3.144108300	-1.045780500	0.065303400
C	3.131987600	0.359808700	-0.020454000
C	1.950000700	1.124113700	-0.207396000
C	0.775324000	-0.991524600	-0.232935400
C	1.912905300	-1.728449200	-0.057660000
C	4.469101200	-1.569718300	0.262381700
C	5.407756700	-0.593578400	0.321586400
N	0.773289300	0.388267400	-0.270252600
H	-0.177138000	-1.467009700	-0.346989200
H	1.850341500	-2.798716800	-0.028714100
H	4.688512500	-2.615198600	0.356987200
H	6.461252000	-0.720729000	0.464330100
S	1.966919500	2.812556800	-0.338971100
S	4.751380800	1.022106600	0.131171500
C	-0.547629700	1.039601400	-0.203429800
O	-1.355272000	0.689241600	-1.333828200
C	-1.356700200	0.666300500	1.018710200
H	-0.470538200	2.125588100	-0.222742400
C	-2.729280100	0.727808800	-0.922195300
C	-2.732551700	1.044278400	0.564811100
H	-1.040100800	1.200359700	1.918825700
H	-1.323031400	-0.403787600	1.240652200

H	-3.212596500	1.547825700	-1.458012500
H	-2.864584900	2.120910200	0.701812300
C	-3.418150600	-0.572761700	-1.328201400
H	-4.488473000	-0.524933800	-1.113736900
H	-3.285977000	-0.755946900	-2.397880000
O	-2.880744000	-1.695002000	-0.639006800
H	-2.840915500	-1.447442300	0.300248900
O	-3.752100800	0.372831500	1.294708300
H	-3.544050200	0.495825300	2.236206700
O	3.850504900	5.681922200	-1.944078900
H	3.397225100	4.860850600	-1.806384200
H	4.715937500	5.548119300	-1.581950100
O	4.785917200	2.208921700	3.643170400
H	4.850428400	2.044295100	2.711994200
H	4.009104700	2.741751300	3.746386500
coord_5			
C	3.143623100	-1.055279900	0.067609900
C	3.129499900	0.360842200	-0.020012300
C	1.953766700	1.114016100	-0.204581900
C	0.772957900	-0.993035000	-0.232522200
C	1.915514600	-1.731563400	-0.055090700
C	4.468249900	-1.573855900	0.264219900
C	5.406839400	-0.595904200	0.322089100
N	0.771752000	0.385486200	-0.270327500
H	-0.178724000	-1.469681800	-0.346775600
H	1.849637400	-2.801767800	-0.025261800
H	4.691313500	-2.618488800	0.359669900
H	6.460308100	-0.723867600	0.464199100
S	1.959399500	2.817469200	-0.339305400
S	4.752972900	1.023752800	0.131182600
C	-0.548281500	1.038786200	-0.202801400
O	-1.356218800	0.689776700	-1.333357100
C	-1.357607500	0.665806600	1.019253200
H	-0.471105200	2.124558600	-0.221378900
C	-2.730132900	0.728377400	-0.921624900
C	-2.733232700	1.044667000	0.565405800
H	-1.040703900	1.199556500	1.919460800
H	-1.324506400	-0.404306100	1.241009800
H	-3.213477800	1.548416500	-1.457373200
H	-2.864684300	2.121363800	0.702604900
C	-3.418865500	-0.572204900	-1.327763400
H	-4.489189200	-0.524389300	-1.113393400

H	-3.286595400	-0.755361500	-2.397441700
O	-2.881520100	-1.694479200	-0.638581700
H	-2.840815500	-1.446592600	0.300554600
O	-3.753053300	0.373563000	1.295207300
H	-3.544673300	0.496036400	2.236697400
O	3.849926100	5.682150400	-1.943574400
H	3.399116800	4.859164400	-1.810487400
H	4.715048800	5.549428900	-1.580381000
O	4.791244800	2.207180700	3.643624500
H	4.857129400	2.033950900	2.714113400
H	4.013654900	2.739669500	3.741115700
coord_6			
C	3.143138000	-1.064779300	0.069916400
C	3.127012200	0.361875800	-0.019570600
C	1.957532700	1.103918600	-0.201767900
C	0.770591800	-0.994545400	-0.232109000
C	1.918123800	-1.734677600	-0.052521400
C	4.467398600	-1.577993500	0.266058100
C	5.405922200	-0.598229900	0.322591900
N	0.770214800	0.382704900	-0.270402400
H	-0.180310000	-1.472353900	-0.346562000
H	1.848933400	-2.804818700	-0.021809500
H	4.694114600	-2.621779100	0.362352700
H	6.459364200	-0.727006200	0.464068100
S	1.951879500	2.822381500	-0.339639700
S	4.754565100	1.025398900	0.131193800
C	-0.548933400	1.037970900	-0.202173000
O	-1.357165700	0.690311900	-1.332886000
C	-1.358514700	0.665312700	1.019796200
H	-0.471672200	2.123529100	-0.220015300
C	-2.730985600	0.728945900	-0.921054600
C	-2.733913700	1.045055700	0.566000500
H	-1.041307100	1.198753300	1.920095800
H	-1.325981400	-0.404824700	1.241367400
H	-3.214359000	1.549007200	-1.456733900
H	-2.864783700	2.121817300	0.703397600
C	-3.419580400	-0.571648100	-1.327325400
H	-4.489905400	-0.523844800	-1.113049900
H	-3.287213800	-0.754776100	-2.397003500
O	-2.882296100	-1.693956400	-0.638156600
H	-2.840715400	-1.445742900	0.300860200
O	-3.754005900	0.374294500	1.295706300

H	-3.545296300	0.496247400	2.237188100
O	3.849347400	5.682378600	-1.943069800
H	3.401008600	4.857478200	-1.814590600
H	4.714160200	5.550738500	-1.578811900
O	4.796572400	2.205439800	3.644078600
H	4.863830400	2.023606800	2.716232600
H	4.018205100	2.737587600	3.735844900
coord_7			
C	3.142652800	-1.074278700	0.072222900
C	3.124524400	0.362909300	-0.019129000
C	1.961298800	1.093821000	-0.198953800
C	0.768225700	-0.996055900	-0.231695800
C	1.920733100	-1.737791800	-0.049952000
C	4.466547200	-1.582131100	0.267896300
C	5.405004900	-0.600555700	0.323094700
N	0.768677500	0.379923700	-0.270477200
H	-0.181896000	-1.475026000	-0.346348300
H	1.848229400	-2.807869700	-0.018357200
H	4.696915600	-2.625069400	0.365035400
H	6.458420300	-0.730144800	0.463937100
S	1.944359500	2.827293900	-0.339974000
S	4.756157200	1.027045000	0.131205000
C	-0.549585200	1.037155600	-0.201544600
O	-1.358112600	0.690847000	-1.332415000
C	-1.359422000	0.664818800	1.020339200
H	-0.472239200	2.122499600	-0.218651800
C	-2.731838400	0.729514400	-0.920484300
C	-2.734594700	1.045444400	0.566595100
H	-1.041910300	1.197950100	1.920730900
H	-1.327456400	-0.405343200	1.241725000
H	-3.215240200	1.549598000	-1.456094600
H	-2.864883100	2.122270800	0.704190300
C	-3.420295300	-0.571091300	-1.326887400
H	-4.490621700	-0.523300400	-1.112706500
H	-3.287832200	-0.754190700	-2.396565300
O	-2.883072200	-1.693433500	-0.637731400
H	-2.840615300	-1.444893200	0.301165800
O	-3.754958500	0.375026000	1.296205300
H	-3.545919400	0.496458500	2.237678700
O	3.848768600	5.682606800	-1.942565300
H	3.402900300	4.855791900	-1.818693900
H	4.713271600	5.552048100	-1.577242800

O	4.801900100	2.203698800	3.644532700
H	4.870531500	2.013262600	2.718351700
H	4.022755300	2.735505800	3.730574000
coord_8			
C	3.142167600	-1.083778100	0.074529400
C	3.122036700	0.363942800	-0.018687300
C	1.965064800	1.083723500	-0.196139800
C	0.765859700	-0.997566300	-0.231282600
C	1.923342300	-1.740906100	-0.047382700
C	4.465695900	-1.586268700	0.269734500
C	5.404087600	-0.602881400	0.323597400
N	0.767140200	0.377142500	-0.270552100
H	-0.183482000	-1.477698100	-0.346134700
H	1.847525400	-2.810920700	-0.014904900
H	4.699716700	-2.628359700	0.367718100
H	6.457476400	-0.733283400	0.463806100
S	1.936839400	2.832206200	-0.340308300
S	4.757749300	1.028691100	0.131216100
C	-0.550237100	1.036340300	-0.200916200
O	-1.359059400	0.691382100	-1.331943900
C	-1.360329300	0.664325000	1.020882100
H	-0.472806200	2.121470100	-0.217288200
C	-2.732691200	0.730083000	-0.919914000
C	-2.735275600	1.045833100	0.567189800
H	-1.042513400	1.197146900	1.921366000
H	-1.328931400	-0.405861700	1.242082700
H	-3.216121400	1.550188700	-1.455455300
H	-2.864982500	2.122724400	0.704983000
C	-3.421010200	-0.570534500	-1.326449400
H	-4.491337900	-0.522755900	-1.112363000
H	-3.288450600	-0.753605300	-2.396127000
O	-2.883848300	-1.692910700	-0.637306300
H	-2.840515200	-1.444043500	0.301471400
O	-3.755911000	0.375757500	1.296704300
H	-3.546542400	0.496669600	2.238169400
O	3.848189900	5.682835000	-1.942060800
H	3.404792000	4.854105700	-1.822797100
H	4.712383000	5.553357700	-1.575673700
O	4.807227700	2.201957800	3.644986800
H	4.877232500	2.002918400	2.720470900
H	4.027305500	2.733424000	3.725303200
coord_9			

C	3.141682400	-1.093277500	0.076835800
C	3.119548900	0.364976400	-0.018245600
C	1.968830900	1.073626000	-0.193325800
C	0.763493600	-0.999076700	-0.230869400
C	1.925951600	-1.744020300	-0.044813400
C	4.464844600	-1.590406300	0.271572700
C	5.403170400	-0.605207200	0.324100200
N	0.765602900	0.374361200	-0.270626900
H	-0.185068000	-1.480370200	-0.345921100
H	1.846821300	-2.813971700	-0.011452600
H	4.702517700	-2.631649900	0.370400800
H	6.456532400	-0.736422000	0.463675200
S	1.929319400	2.837118500	-0.340642700
S	4.759341500	1.030337300	0.131227300
C	-0.550888900	1.035525000	-0.200287800
O	-1.360006300	0.691917300	-1.331472800
C	-1.361236600	0.663831100	1.021425100
H	-0.473373200	2.120440600	-0.215924700
C	-2.733543900	0.730651500	-0.919343600
C	-2.735956600	1.046221800	0.567784500
H	-1.043116600	1.196343600	1.922001000
H	-1.330406400	-0.406380200	1.242440300
H	-3.217002600	1.550779500	-1.454816100
H	-2.865081800	2.123177900	0.705775700
C	-3.421725000	-0.569977700	-1.326011500
H	-4.492054100	-0.522211500	-1.112019500
H	-3.289068900	-0.753019800	-2.395688800
O	-2.884624300	-1.692387900	-0.636881200
H	-2.840415100	-1.443193700	0.301777000
O	-3.756863600	0.376488900	1.297203200
H	-3.547165500	0.496880600	2.238660100
O	3.847611200	5.683063200	-1.941556200
H	3.406683700	4.852419400	-1.826900300
H	4.711494300	5.554667300	-1.574104600
O	4.812555300	2.200216800	3.645441000
H	4.883933500	1.992574300	2.722590000
H	4.031855700	2.731342200	3.720032400

coord_10

C	3.141197200	-1.102776800	0.079142300
C	3.117061200	0.366009900	-0.017804000
C	1.972596900	1.063528400	-0.190511700
C	0.761127500	-1.000587100	-0.230456200

C	1.928560800	-1.747134500	-0.042244100
C	4.463993200	-1.594543900	0.273410900
C	5.402253100	-0.607533000	0.324603000
N	0.764065600	0.371580000	-0.270701800
H	-0.186654000	-1.483042300	-0.345707500
H	1.846117300	-2.817022700	-0.008000300
H	4.705318800	-2.634940200	0.373083500
H	6.455588500	-0.739560600	0.463544200
S	1.921799400	2.842030900	-0.340977000
S	4.760933600	1.031983400	0.131238400
C	-0.551540800	1.034709800	-0.199659300
O	-1.360953100	0.692452400	-1.331001800
C	-1.362143800	0.663337200	1.021968100
H	-0.473940300	2.119411100	-0.214561100
C	-2.734396700	0.731220100	-0.918773300
C	-2.736637600	1.046610500	0.568379100
H	-1.043719800	1.195540400	1.922636100
H	-1.331881400	-0.406898700	1.242797900
H	-3.217883800	1.551370200	-1.454176800
H	-2.865181200	2.123631500	0.706568400
C	-3.422439900	-0.569420800	-1.325573500
H	-4.492770400	-0.521667000	-1.111676000
H	-3.289687300	-0.752434400	-2.395250600
O	-2.885400400	-1.691865100	-0.636456100
H	-2.840315000	-1.442344000	0.302082700
O	-3.757816200	0.377220400	1.297702200
H	-3.547788600	0.497091700	2.239150800
O	3.847032400	5.683291400	-1.941051700
H	3.408575400	4.850733200	-1.831003500
H	4.710605700	5.555976900	-1.572535500
O	4.817882900	2.198475900	3.645895100
H	4.890634500	1.982230100	2.724709200
H	4.036405900	2.729260300	3.714761500

S₂(¹ππ*) minimum to S₁(¹nπ*) minimum

coord_1

C	3.141197200	-1.102776800	0.079142300
C	3.117061200	0.366009900	-0.017804000
C	1.972596900	1.063528400	-0.190511700
C	0.761127500	-1.000587100	-0.230456200
C	1.928560800	-1.747134500	-0.042244100
C	4.463993200	-1.594543900	0.273410900
C	5.402253100	-0.607533000	0.324603000

N	0.764065600	0.371580000	-0.270701800
H	-0.186654000	-1.483042300	-0.345707500
H	1.846117300	-2.817022700	-0.008000300
H	4.705318800	-2.634940200	0.373083500
H	6.455588500	-0.739560600	0.463544200
S	1.921799400	2.842030900	-0.340977000
S	4.760933600	1.031983400	0.131238400
C	-0.551540800	1.034709800	-0.199659300
O	-1.360953100	0.692452400	-1.331001800
C	-1.362143800	0.663337200	1.021968100
H	-0.473940300	2.119411100	-0.214561100
C	-2.734396700	0.731220100	-0.918773300
C	-2.736637600	1.046610500	0.568379100
H	-1.043719800	1.195540400	1.922636100
H	-1.331881400	-0.406898700	1.242797900
H	-3.217883800	1.551370200	-1.454176800
H	-2.865181200	2.123631500	0.706568400
C	-3.422439900	-0.569420800	-1.325573500
H	-4.492770400	-0.521667000	-1.111676000
H	-3.289687300	-0.752434400	-2.395250600
O	-2.885400400	-1.691865100	-0.636456100
H	-2.840315000	-1.442344000	0.302082700
O	-3.757816200	0.377220400	1.297702200
H	-3.547788600	0.497091700	2.239150800
O	3.847032400	5.683291400	-1.941051700
H	3.408575400	4.850733200	-1.831003500
H	4.710605700	5.555976900	-1.572535500
O	4.817882900	2.198475900	3.645895100
H	4.890634500	1.982230100	2.724709200
H	4.036405900	2.729260300	3.714761500

coord_2

C	3.144121000	-1.096223000	0.081898000
C	3.119019000	0.368349000	-0.014807000
C	1.973652000	1.066673000	-0.190081000
C	0.763791000	-1.001430000	-0.232650000
C	1.927355000	-1.744526000	-0.044761000
C	4.465186000	-1.589728000	0.275873000
C	5.406478000	-0.604198000	0.327671000
N	0.763276000	0.373968000	-0.267816000
H	-0.183673000	-1.483719000	-0.351819000
H	1.848277000	-2.814678000	-0.014796000
H	4.704613000	-2.630660000	0.374806000

H	6.459717000	-0.735416000	0.466980000
S	1.932304000	2.843970000	-0.344314000
S	4.762410000	1.033332000	0.135130000
C	-0.550915000	1.037657000	-0.193608000
O	-1.360451000	0.700786000	-1.326331000
C	-1.361493000	0.661040000	1.026205000
H	-0.469990000	2.122256000	-0.203676000
C	-2.733883000	0.736125000	-0.913714000
C	-2.735949000	1.046451000	0.574355000
H	-1.042831000	1.188875000	1.929242000
H	-1.331204000	-0.410166000	1.241921000
H	-3.218749000	1.557273000	-1.446306000
H	-2.864013000	2.123001000	0.716112000
C	-3.420440000	-0.564094000	-1.324470000
H	-4.490924000	-0.517991000	-1.110938000
H	-3.287080000	-0.743984000	-2.394548000
O	-2.882698000	-1.688013000	-0.638377000
H	-2.839598000	-1.441767000	0.301049000
O	-3.757436000	0.375125000	1.301396000
H	-3.548808000	0.493958000	2.243281000
O	3.834996000	5.669430000	-1.938626000
H	3.411732000	4.823047000	-1.893981000
H	4.701719000	5.542349000	-1.578297000
O	4.824252000	2.201769000	3.651065000
H	4.893514000	1.964824000	2.736925000
H	4.037288000	2.724084000	3.714447000

coord_3

C	3.147019000	-1.089546000	0.084570000
C	3.120950000	0.370811000	-0.011904000
C	1.974679000	1.069937000	-0.189748000
C	0.766429000	-1.002155000	-0.234929000
C	1.926126000	-1.741797000	-0.047357000
C	4.466355000	-1.584786000	0.278255000
C	5.410677000	-0.600736000	0.330653000
N	0.762460000	0.376474000	-0.265025000
H	-0.180717000	-1.484281000	-0.358013000
H	1.850415000	-2.812213000	-0.021665000
H	4.703885000	-2.626254000	0.376455000
H	6.463819000	-0.731143000	0.470331000
S	1.942779000	2.846027000	-0.347761000
S	4.763858000	1.034805000	0.138926000
C	-0.550317000	1.040720000	-0.187655000

O	-1.359975000	0.709227000	-1.321756000
C	-1.360869000	0.658864000	1.030345000
H	-0.466070000	2.125216000	-0.192896000
C	-2.733397000	0.741139000	-0.908752000
C	-2.735288000	1.046409000	0.580232000
H	-1.041970000	1.182337000	1.935748000
H	-1.330553000	-0.413309000	1.240955000
H	-3.219643000	1.563279000	-1.438537000
H	-2.862875000	2.122489000	0.725551000
C	-3.418465000	-0.558662000	-1.323456000
H	-4.489103000	-0.514211000	-1.110289000
H	-3.284497000	-0.735435000	-2.393934000
O	-2.880018000	-1.684051000	-0.640380000
H	-2.838905000	-1.441075000	0.299933000
O	-3.757082000	0.373149000	1.304994000
H	-3.549856000	0.490951000	2.247316000
O	3.822925000	5.655680000	-1.936326000
H	3.417831000	4.799614000	-1.960002000
H	4.693155000	5.528783000	-1.584038000
O	4.830591000	2.205210000	3.656131000
H	4.896363000	1.947560000	2.749038000
H	4.038140000	2.719053000	3.714024000
coord_4			
C	0.769068000	-1.002881000	-0.237207000
C	1.924897000	-1.739068000	-0.049954000
C	4.467524000	-1.579844000	0.280637000
C	5.414876000	-0.597274000	0.333634000
N	0.761644000	0.378979000	-0.262233000
H	-0.177760000	-1.484842000	-0.364208000
H	1.852553000	-2.809748000	-0.028534000
H	4.703156000	-2.621848000	0.378104000
H	6.467922000	-0.726869000	0.473682000
S	1.953254000	2.848085000	-0.351207000
S	4.765306000	1.036278000	0.142721000
C	-0.549719000	1.043782000	-0.181702000
O	-1.359500000	0.717667000	-1.317181000
C	-1.360245000	0.656689000	1.034485000
H	-0.462149000	2.128176000	-0.182116000
C	-2.732910000	0.746152000	-0.903791000
C	-2.734627000	1.046367000	0.586108000
H	-1.041109000	1.175799000	1.942254000
H	-1.329902000	-0.416453000	1.239989000

H	-3.220537000	1.569286000	-1.430768000
H	-2.861736000	2.121976000	0.734989000
C	-3.416490000	-0.553230000	-1.322442000
H	-4.487282000	-0.510431000	-1.109641000
H	-3.281915000	-0.726887000	-2.393319000
O	-2.877339000	-1.680089000	-0.642383000
H	-2.838212000	-1.440383000	0.298816000
O	-3.756728000	0.371173000	1.308593000
H	-3.550903000	0.487944000	2.251351000
O	3.810855000	5.641929000	-1.934027000
H	3.426874000	4.780968000	-2.027919000
H	4.684367000	5.515251000	-1.589877000
O	4.836931000	2.208651000	3.661197000
H	4.899424000	1.929349000	2.758094000
H	4.038991000	2.714023000	3.713602000
coord_5			
C	3.152816000	-1.076193000	0.089913000
C	3.124812000	0.375734000	-0.006096000
C	1.976734000	1.076464000	-0.189081000
C	0.771707000	-1.003606000	-0.239486000
C	1.923668000	-1.736339000	-0.052551000
C	4.468693000	-1.574902000	0.283019000
C	5.419075000	-0.593812000	0.336616000
N	0.760828000	0.381484000	-0.259441000
H	-0.174803000	-1.485404000	-0.370402000
H	1.854691000	-2.807284000	-0.035403000
H	4.702428000	-2.617441000	0.379753000
H	6.472025000	-0.722595000	0.477033000
S	1.963728000	2.850142000	-0.354653000
S	4.766754000	1.037751000	0.146516000
C	-0.549121000	1.046845000	-0.175750000
O	-1.359024000	0.726108000	-1.312606000
C	-1.359622000	0.654513000	1.038626000
H	-0.458229000	2.131137000	-0.171336000
C	-2.732423000	0.751165000	-0.898829000
C	-2.733967000	1.046325000	0.591985000
H	-1.040249000	1.169261000	1.948760000
H	-1.329250000	-0.419596000	1.239023000
H	-3.221430000	1.575293000	-1.422999000
H	-2.860598000	2.121464000	0.744427000
C	-3.414515000	-0.547798000	-1.321427000
H	-4.485461000	-0.506652000	-1.108992000

H	-3.279332000	-0.718338000	-2.392705000
O	-2.874660000	-1.676128000	-0.644385000
H	-2.837519000	-1.439691000	0.297699000
O	-3.756375000	0.369198000	1.312191000
H	-3.551951000	0.484937000	2.255386000
O	3.798784000	5.628179000	-1.931727000
H	3.438667000	4.767555000	-2.096508000
H	4.675503000	5.501729000	-1.595746000
O	4.843269000	2.212091000	3.666263000
H	4.902276000	1.911946000	2.770026000
H	4.039843000	2.708993000	3.713179000
coord_6			
C	3.155715000	-1.069517000	0.092585000
C	3.126743000	0.378195000	-0.003193000
C	1.977761000	1.079728000	-0.188748000
C	0.774345000	-1.004332000	-0.241765000
C	1.922439000	-1.733611000	-0.055148000
C	4.469861000	-1.569960000	0.285401000
C	5.423274000	-0.590349000	0.339598000
N	0.760011000	0.383989000	-0.256649000
H	-0.171846000	-1.485965000	-0.376596000
H	1.856828000	-2.804819000	-0.042271000
H	4.701699000	-2.613035000	0.381402000
H	6.476128000	-0.718321000	0.480383000
S	1.974203000	2.852199000	-0.358100000
S	4.768202000	1.039225000	0.150312000
C	-0.548523000	1.049907000	-0.169797000
O	-1.358548000	0.734549000	-1.308031000
C	-1.358998000	0.652338000	1.042766000
H	-0.454308000	2.134097000	-0.160556000
C	-2.731937000	0.756178000	-0.893867000
C	-2.733306000	1.046282000	0.597862000
H	-1.039388000	1.162724000	1.955266000
H	-1.328599000	-0.422740000	1.238057000
H	-3.222324000	1.581299000	-1.415230000
H	-2.859459000	2.120951000	0.753865000
C	-3.412539000	-0.542367000	-1.320413000
H	-4.483640000	-0.502872000	-1.108343000
H	-3.276749000	-0.709790000	-2.392091000
O	-2.871981000	-1.672166000	-0.646388000
H	-2.836826000	-1.438998000	0.296582000
O	-3.756021000	0.367222000	1.315790000

H	-3.552998000	0.481930000	2.259421000
O	3.786714000	5.614428000	-1.929427000
H	3.452851000	4.759552000	-2.164444000
H	4.666566000	5.488219000	-1.601645000
O	4.849609000	2.215532000	3.671329000
H	4.905116000	1.894584000	2.782104000
H	4.040694000	2.703963000	3.712757000
coord_7			
C	3.158613000	-1.062840000	0.095256000
C	3.128674000	0.380656000	-0.000289000
C	1.978788000	1.082992000	-0.188415000
C	0.776984000	-1.005057000	-0.244044000
C	1.921210000	-1.730882000	-0.057744000
C	4.471030000	-1.565019000	0.287783000
C	5.427474000	-0.586887000	0.342579000
N	0.759195000	0.386494000	-0.253858000
H	-0.168889000	-1.486527000	-0.382790000
H	1.858966000	-2.802354000	-0.049140000
H	4.700971000	-2.608629000	0.383051000
H	6.480231000	-0.714047000	0.483734000
S	1.984678000	2.854257000	-0.361546000
S	4.769651000	1.040698000	0.154107000
C	-0.547925000	1.052970000	-0.163844000
O	-1.358073000	0.742990000	-1.303456000
C	-1.358375000	0.650162000	1.046906000
H	-0.450388000	2.137057000	-0.149776000
C	-2.731450000	0.761191000	-0.888905000
C	-2.732645000	1.046240000	0.603738000
H	-1.038528000	1.156186000	1.961772000
H	-1.327948000	-0.425884000	1.237091000
H	-3.223218000	1.587306000	-1.407461000
H	-2.858321000	2.120439000	0.763304000
C	-3.410564000	-0.536935000	-1.319399000
H	-4.481818000	-0.499092000	-1.107695000
H	-3.274166000	-0.701241000	-2.391476000
O	-2.869302000	-1.668204000	-0.648391000
H	-2.836133000	-1.438306000	0.295466000
O	-3.755668000	0.365247000	1.319388000
H	-3.554046000	0.478924000	2.263455000
O	3.774644000	5.600678000	-1.927128000
H	3.468929000	4.756838000	-2.230413000
H	4.657552000	5.474718000	-1.607570000

O	4.855948000	2.218973000	3.676395000
H	4.907928000	1.877408000	2.794669000
H	4.041545000	2.698933000	3.712334000
coord_8			
C	3.161512000	-1.056164000	0.097928000
C	3.130605000	0.383118000	0.002615000
C	1.979816000	1.086256000	-0.188082000
C	0.779623000	-1.005783000	-0.246323000
C	1.919981000	-1.728153000	-0.060341000
C	4.472199000	-1.560077000	0.290165000
C	5.431673000	-0.583425000	0.345561000
N	0.758379000	0.388999000	-0.251066000
H	-0.165933000	-1.487089000	-0.388985000
H	1.861104000	-2.799889000	-0.056009000
H	4.700243000	-2.604222000	0.384700000
H	6.484334000	-0.709773000	0.487085000
S	1.995152000	2.856314000	-0.364992000
S	4.771099000	1.042171000	0.157903000
C	-0.547327000	1.056032000	-0.157891000
O	-1.357597000	0.751430000	-1.298881000
C	-1.357751000	0.647987000	1.051047000
H	-0.446467000	2.140018000	-0.138996000
C	-2.730964000	0.766204000	-0.883943000
C	-2.731984000	1.046198000	0.609615000
H	-1.037667000	1.149648000	1.968278000
H	-1.327297000	-0.429027000	1.236125000
H	-3.224111000	1.593312000	-1.399692000
H	-2.857182000	2.119926000	0.772742000
C	-3.408589000	-0.531504000	-1.318384000
H	-4.479997000	-0.495312000	-1.107046000
H	-3.271584000	-0.692693000	-2.390862000
O	-2.866623000	-1.664243000	-0.650394000
H	-2.835441000	-1.437614000	0.294349000
O	-3.755314000	0.363271000	1.322987000
H	-3.555093000	0.475917000	2.267490000
O	3.762573000	5.586927000	-1.924828000
H	3.486309000	4.759001000	-2.293239000
H	4.648193000	5.461267000	-1.613616000
O	4.862287000	2.222413000	3.681461000
H	4.910611000	1.861238000	2.809604000
H	4.042397000	2.693902000	3.711912000

coord_9

C	3.164410000	-1.049487000	0.100600000
C	3.132536000	0.385579000	0.005518000
C	1.980843000	1.089520000	-0.187749000
C	0.782261000	-1.006508000	-0.248601000
C	1.918752000	-1.725424000	-0.062938000
C	4.473368000	-1.555135000	0.292546000
C	5.435872000	-0.579963000	0.348543000
N	0.757563000	0.391504000	-0.248274000
H	-0.162976000	-1.487650000	-0.395179000
H	1.863241000	-2.797424000	-0.062878000
H	4.699514000	-2.599816000	0.386349000
H	6.488436000	-0.705499000	0.490436000
S	2.005627000	2.858371000	-0.368439000
S	4.772547000	1.043644000	0.161698000
C	-0.546729000	1.059095000	-0.151938000
O	-1.357121000	0.759871000	-1.294306000
C	-1.357127000	0.645811000	1.055187000
H	-0.442547000	2.142978000	-0.128216000
C	-2.730477000	0.771217000	-0.878981000
C	-2.731323000	1.046156000	0.615491000
H	-1.036807000	1.143110000	1.974784000
H	-1.326645000	-0.432171000	1.235159000
H	-3.225005000	1.599319000	-1.391923000
H	-2.856044000	2.119414000	0.782180000
C	-3.406614000	-0.526072000	-1.317370000
H	-4.478176000	-0.491532000	-1.106397000
H	-3.269001000	-0.684144000	-2.390247000
O	-2.863944000	-1.660281000	-0.652397000
H	-2.834748000	-1.436922000	0.293232000
O	-3.754961000	0.361296000	1.326585000
H	-3.556141000	0.472910000	2.271525000
O	3.750503000	5.573177000	-1.922528000
H	3.504367000	4.765402000	-2.351976000
H	4.639273000	5.447754000	-1.619502000
O	4.868626000	2.225854000	3.686527000
H	4.913461000	1.843973000	2.821718000
H	4.043248000	2.688872000	3.711490000

coord_10

C	3.168010000	-1.042290000	0.103688000
C	3.135126000	0.388565000	0.008919000
C	1.982508000	1.093285000	-0.186874000
C	0.785599000	-1.006763000	-0.250452000

C	1.918243000	-1.722202000	-0.065151000
C	4.475253000	-1.549645000	0.295311000
C	5.440759000	-0.575928000	0.351958000
N	0.757405000	0.394479000	-0.244975000
H	-0.159306000	-1.487760000	-0.400968000
H	1.866131000	-2.794467000	-0.069424000
H	4.699533000	-2.594860000	0.388321000
H	6.493231000	-0.700630000	0.494209000
S	2.016687000	2.860941000	-0.371244000
S	4.774635000	1.045681000	0.166021000
C	-0.545491000	1.062583000	-0.145435000
O	-1.356002000	0.768778000	-1.289194000
C	-1.355847000	0.643970000	1.059857000
H	-0.438018000	2.146365000	-0.116825000
C	-2.729345000	0.776633000	-0.873476000
C	-2.730019000	1.046432000	0.621926000
H	-1.035300000	1.136864000	1.981846000
H	-1.325305000	-0.434989000	1.234662000
H	-3.225279000	1.605742000	-1.383562000
H	-2.854292000	2.119206000	0.792237000
C	-3.403957000	-0.520232000	-1.315883000
H	-4.475673000	-0.487387000	-1.105270000
H	-3.265736000	-0.675123000	-2.389169000
O	-2.860547000	-1.655932000	-0.653993000
H	-2.833340000	-1.435895000	0.292534000
O	-3.753940000	0.359569000	1.330707000
H	-3.556521000	0.470104000	2.276088000
O	3.738932000	5.560076000	-1.919442000
H	3.522233000	4.773061000	-2.406992000
H	4.630856000	5.434899000	-1.624613000
O	4.875584000	2.229662000	3.692186000
H	4.916938000	1.827126000	2.834401000
H	4.044706000	2.684184000	3.711689000

S₂(¹ππ*) minimum to T₂(³nπ*) minimum

coord_1

C	3.141221000	-1.102899000	0.079226000
C	3.117087000	0.365888000	-0.017711000
C	1.972624000	1.063409000	-0.190414000
C	0.761152000	-1.000704000	-0.230371000
C	1.928584000	-1.747254000	-0.042164000
C	4.464016000	-1.594669000	0.273491000
C	5.402277000	-0.607660000	0.324689000

N	0.764092000	0.371463000	-0.270608000
H	-0.186630000	-1.483157000	-0.345625000
H	1.846139000	-2.817142000	-0.007927000
H	4.705340000	-2.635066000	0.373157000
H	6.455612000	-0.739690000	0.463629000
S	1.921829000	2.841912000	-0.340868000
S	4.760960000	1.031858000	0.131335000
C	-0.551513000	1.034594000	-0.199561000
O	-1.360926000	0.692345000	-1.330905000
C	-1.362116000	0.663215000	1.022064000
H	-0.473911000	2.119295000	-0.214456000
C	-2.734369000	0.731112000	-0.918676000
C	-2.736609000	1.046493000	0.568478000
H	-1.043691000	1.195412000	1.922735000
H	-1.331855000	-0.407022000	1.242887000
H	-3.217855000	1.551266000	-1.454074000
H	-2.865151000	2.123513000	0.706674000
C	-3.422414000	-0.569525000	-1.325484000
H	-4.492744000	-0.521771000	-1.111586000
H	-3.289662000	-0.752532000	-2.395162000
O	-2.885376000	-1.691974000	-0.636374000
H	-2.840290000	-1.442459000	0.302166000
O	-3.757788000	0.377100000	1.297797000
H	-3.547760000	0.496965000	2.239246000
O	3.847065000	5.683179000	-1.940925000
H	3.408607000	4.850621000	-1.830882000
H	4.710638000	5.555861000	-1.572410000
O	4.817912000	2.198328000	3.645998000
H	4.890663000	1.982088000	2.724811000
H	4.036436000	2.729113000	3.714868000

coord_2

C	3.142648000	-1.096660000	0.086892000
C	3.118787000	0.366553000	-0.013656000
C	1.973254000	1.065537000	-0.190220000
C	0.762668000	-1.001535000	-0.230422000
C	1.925886000	-1.745135000	-0.042388000
C	4.464343000	-1.590556000	0.281344000
C	5.405484000	-0.605900000	0.329222000
N	0.761913000	0.373719000	-0.258593000
H	-0.184859000	-1.483146000	-0.351114000
H	1.847036000	-2.815276000	-0.014639000
H	4.703552000	-2.631307000	0.382833000

H	6.458803000	-0.737143000	0.468008000
S	1.931765000	2.840048000	-0.362250000
S	4.762063000	1.031288000	0.132465000
C	-0.550737000	1.038520000	-0.177279000
O	-1.361400000	0.712981000	-1.311662000
C	-1.361314000	0.653261000	1.039159000
H	-0.466902000	2.122271000	-0.177551000
C	-2.734566000	0.745233000	-0.898115000
C	-2.735289000	1.044082000	0.591573000
H	-1.041577000	1.173056000	1.945718000
H	-1.332533000	-0.419056000	1.246095000
H	-3.219831000	1.569998000	-1.423943000
H	-2.861430000	2.119209000	0.741689000
C	-3.422041000	-0.551178000	-1.317882000
H	-4.492230000	-0.506562000	-1.102642000
H	-3.290318000	-0.722692000	-2.389060000
O	-2.883829000	-1.680052000	-0.641498000
H	-2.838941000	-1.440968000	0.299272000
O	-3.757297000	0.368932000	1.313838000
H	-3.546034000	0.477164000	2.255843000
O	3.828561000	5.667217000	-1.920676000
H	3.408450000	4.820200000	-1.898023000
H	4.698362000	5.550706000	-1.568092000
O	4.826209000	2.203638000	3.651810000
H	4.896231000	1.971477000	2.735622000
H	4.039306000	2.725985000	3.716839000
coord_3			
C	3.144074000	-1.090421000	0.094557000
C	3.120486000	0.367217000	-0.009600000
C	1.973883000	1.067664000	-0.190027000
C	0.764183000	-1.002366000	-0.230474000
C	1.923188000	-1.743015000	-0.042611000
C	4.464669000	-1.586443000	0.289198000
C	5.408690000	-0.604139000	0.333756000
N	0.759734000	0.375976000	-0.246578000
H	-0.183087000	-1.483134000	-0.356604000
H	1.847932000	-2.813410000	-0.021350000
H	4.701762000	-2.627548000	0.392509000
H	6.461992000	-0.734597000	0.472386000
S	1.941700000	2.838184000	-0.383633000
S	4.763164000	1.030718000	0.133595000
C	-0.549960000	1.042446000	-0.154998000

O	-1.361873000	0.733616000	-1.292418000
C	-1.360512000	0.643308000	1.056253000
H	-0.459893000	2.125246000	-0.140645000
C	-2.734762000	0.759354000	-0.877555000
C	-2.733968000	1.041671000	0.614668000
H	-1.039463000	1.150701000	1.968700000
H	-1.333210000	-0.431089000	1.249302000
H	-3.221805000	1.588729000	-1.393812000
H	-2.857708000	2.114904000	0.776703000
C	-3.421667000	-0.532832000	-1.310280000
H	-4.491714000	-0.491353000	-1.093697000
H	-3.290972000	-0.692851000	-2.382958000
O	-2.882281000	-1.668130000	-0.646622000
H	-2.837592000	-1.439476000	0.296379000
O	-3.756805000	0.360764000	1.329879000
H	-3.544307000	0.457364000	2.272440000
O	3.810056000	5.651253000	-1.900427000
H	3.413085000	4.795188000	-1.972558000
H	4.687900000	5.545331000	-1.563076000
O	4.834505000	2.208947000	3.657621000
H	4.901798000	1.960865000	2.746433000
H	4.042174000	2.722857000	3.718809000
coord_4			
C	3.145500000	-1.084181000	0.102223000
C	3.122186000	0.367881000	-0.005545000
C	1.974512000	1.069791000	-0.189833000
C	0.765698000	-1.003197000	-0.230525000
C	1.920489000	-1.740896000	-0.042835000
C	4.464995000	-1.582330000	0.297051000
C	5.411895000	-0.602379000	0.338289000
N	0.757555000	0.378232000	-0.234562000
H	-0.181315000	-1.483122000	-0.362093000
H	1.848828000	-2.811543000	-0.028062000
H	4.699973000	-2.623788000	0.402185000
H	6.465182000	-0.732050000	0.476764000
S	1.951635000	2.836320000	-0.405015000
S	4.764265000	1.030147000	0.134725000
C	-0.549184000	1.046372000	-0.132716000
O	-1.362346000	0.754251000	-1.273174000
C	-1.359709000	0.633354000	1.073347000
H	-0.452884000	2.128221000	-0.103740000
C	-2.734958000	0.773475000	-0.856994000

C	-2.732648000	1.039260000	0.637763000
H	-1.037349000	1.128345000	1.991682000
H	-1.333888000	-0.443122000	1.252510000
H	-3.223780000	1.607460000	-1.363681000
H	-2.853986000	2.110600000	0.811718000
C	-3.421293000	-0.514485000	-1.302677000
H	-4.491199000	-0.476145000	-1.084752000
H	-3.291627000	-0.663011000	-2.376856000
O	-2.880733000	-1.656208000	-0.651745000
H	-2.836243000	-1.437984000	0.293485000
O	-3.756314000	0.352596000	1.345919000
H	-3.542580000	0.437563000	2.289037000
O	3.791551000	5.635289000	-1.880178000
H	3.424160000	4.780281000	-2.052283000
H	4.676475000	5.540107000	-1.558486000
O	4.842800000	2.214256000	3.663432000
H	4.907364000	1.950253000	2.757243000
H	4.045043000	2.719729000	3.720778000
coord_5			
C	3.146926000	-1.077942000	0.109888000
C	3.123885000	0.368546000	-0.001490000
C	1.975142000	1.071918000	-0.189640000
C	0.767213000	-1.004027000	-0.230576000
C	1.917790000	-1.738776000	-0.043058000
C	4.465321000	-1.578217000	0.304904000
C	5.415101000	-0.600619000	0.342822000
N	0.755375000	0.380488000	-0.222547000
H	-0.179544000	-1.483111000	-0.367582000
H	1.849724000	-2.809677000	-0.034773000
H	4.698183000	-2.620029000	0.411861000
H	6.468371000	-0.729503000	0.481142000
S	1.961570000	2.834455000	-0.426398000
S	4.765366000	1.029577000	0.135856000
C	-0.548408000	1.050298000	-0.110434000
O	-1.362819000	0.774887000	-1.253930000
C	-1.358907000	0.623400000	1.090442000
H	-0.445875000	2.131196000	-0.066834000
C	-2.735154000	0.787596000	-0.836433000
C	-2.731327000	1.036849000	0.660858000
H	-1.035235000	1.105989000	2.014664000
H	-1.334565000	-0.455156000	1.255718000
H	-3.225754000	1.626192000	-1.333550000

H	-2.850264000	2.106295000	0.846733000
C	-3.420918000	-0.496138000	-1.295075000
H	-4.490683000	-0.460936000	-1.075807000
H	-3.292282000	-0.633170000	-2.370753000
O	-2.879185000	-1.644286000	-0.656869000
H	-2.834894000	-1.436492000	0.290591000
O	-3.755822000	0.344429000	1.361960000
H	-3.540853000	0.417762000	2.305633000
O	3.773046000	5.619326000	-1.859929000
H	3.441136000	4.776419000	-2.133753000
H	4.664652000	5.534942000	-1.554066000
O	4.851096000	2.219565000	3.669243000
H	4.912931000	1.939641000	2.768053000
H	4.047911000	2.716600000	3.722748000
coord_6			
C	3.148352000	-1.071703000	0.117554000
C	3.125584000	0.369210000	0.002565000
C	1.975771000	1.074046000	-0.189446000
C	0.768729000	-1.004858000	-0.230627000
C	1.915092000	-1.736656000	-0.043282000
C	4.465647000	-1.574104000	0.312758000
C	5.418307000	-0.598858000	0.347356000
N	0.753196000	0.382745000	-0.210532000
H	-0.177772000	-1.483099000	-0.373072000
H	1.850620000	-2.807810000	-0.041485000
H	4.696394000	-2.616269000	0.421537000
H	6.471560000	-0.726957000	0.485521000
S	1.971505000	2.832591000	-0.447780000
S	4.766468000	1.029007000	0.136986000
C	-0.547631000	1.054224000	-0.088152000
O	-1.363292000	0.795522000	-1.234686000
C	-1.358104000	0.613446000	1.107536000
H	-0.438866000	2.134171000	-0.029929000
C	-2.735349000	0.801717000	-0.815873000
C	-2.730006000	1.034439000	0.683953000
H	-1.033121000	1.083633000	2.037647000
H	-1.335243000	-0.467189000	1.258925000
H	-3.227729000	1.644923000	-1.303419000
H	-2.846542000	2.101990000	0.881747000
C	-3.420544000	-0.477791000	-1.287473000
H	-4.490167000	-0.445727000	-1.066862000
H	-3.292937000	-0.603330000	-2.364651000

O	-2.877637000	-1.632363000	-0.661993000
H	-2.833544000	-1.435001000	0.287697000
O	-3.755330000	0.336261000	1.378001000
H	-3.539127000	0.397961000	2.322230000
O	3.754541000	5.603362000	-1.839680000
H	3.463028000	4.784001000	-2.212914000
H	4.652424000	5.529822000	-1.549795000
O	4.859391000	2.224874000	3.675054000
H	4.918527000	1.928884000	2.778426000
H	4.050779000	2.713472000	3.724718000
coord_7			
C	3.149778000	-1.065464000	0.125219000
C	3.127283000	0.369874000	0.006621000
C	1.976400000	1.076173000	-0.189253000
C	0.770244000	-1.005689000	-0.230679000
C	1.912394000	-1.734537000	-0.043505000
C	4.465973000	-1.569991000	0.320611000
C	5.421512000	-0.597098000	0.351889000
N	0.751017000	0.385001000	-0.198517000
H	-0.176001000	-1.483087000	-0.378561000
H	1.851516000	-2.805944000	-0.048196000
H	4.694604000	-2.612509000	0.431213000
H	6.474749000	-0.724410000	0.489899000
S	1.981440000	2.830726000	-0.469162000
S	4.767569000	1.028437000	0.138116000
C	-0.546855000	1.058150000	-0.065870000
O	-1.363765000	0.816157000	-1.215442000
C	-1.357302000	0.603492000	1.124630000
H	-0.431858000	2.137147000	0.006977000
C	-2.735545000	0.815839000	-0.795312000
C	-2.728685000	1.032028000	0.707048000
H	-1.031007000	1.061278000	2.060629000
H	-1.335920000	-0.479222000	1.262133000
H	-3.229703000	1.663654000	-1.273288000
H	-2.842821000	2.097685000	0.916762000
C	-3.420170000	-0.459444000	-1.279870000
H	-4.489652000	-0.430518000	-1.057917000
H	-3.293591000	-0.573489000	-2.358548000
O	-2.876089000	-1.620441000	-0.667117000
H	-2.832195000	-1.433509000	0.284804000
O	-3.754838000	0.328093000	1.394042000
H	-3.537400000	0.378161000	2.338827000

O	3.736036000	5.587398000	-1.819431000
H	3.488234000	4.802093000	-2.285827000
H	4.639780000	5.524731000	-1.545651000
O	4.867687000	2.230184000	3.680865000
H	4.924065000	1.918417000	2.789674000
H	4.053648000	2.710344000	3.726687000
coord_8			
C	3.151204000	-1.059225000	0.132885000
C	3.128983000	0.370539000	0.010676000
C	1.977029000	1.078300000	-0.189059000
C	0.771759000	-1.006520000	-0.230730000
C	1.909695000	-1.732417000	-0.043729000
C	4.466299000	-1.565877000	0.328464000
C	5.424718000	-0.595337000	0.356422000
N	0.748838000	0.387257000	-0.186502000
H	-0.174229000	-1.483076000	-0.384050000
H	1.852412000	-2.804077000	-0.054908000
H	4.692815000	-2.608750000	0.440889000
H	6.477939000	-0.721863000	0.494278000
S	1.991375000	2.828862000	-0.490545000
S	4.768670000	1.027866000	0.139246000
C	-0.546079000	1.062076000	-0.043589000
O	-1.364238000	0.836793000	-1.196198000
C	-1.356499000	0.593538000	1.141725000
H	-0.424849000	2.140122000	0.043882000
C	-2.735741000	0.829960000	-0.774751000
C	-2.727365000	1.029617000	0.730143000
H	-1.028893000	1.038922000	2.083611000
H	-1.336598000	-0.491256000	1.265340000
H	-3.231678000	1.682386000	-1.243157000
H	-2.839099000	2.093381000	0.951777000
C	-3.419796000	-0.441098000	-1.272268000
H	-4.489136000	-0.415309000	-1.048973000
H	-3.294246000	-0.543649000	-2.352446000
O	-2.874541000	-1.608519000	-0.672241000
H	-2.830846000	-1.432017000	0.281910000
O	-3.754346000	0.319925000	1.410082000
H	-3.535673000	0.358360000	2.355423000
O	3.717531000	5.571434000	-1.799182000
H	3.514839000	4.828604000	-2.349413000
H	4.626713000	5.519655000	-1.541612000
O	4.875982000	2.235493000	3.686676000

H	4.929631000	1.907805000	2.800485000
H	4.056516000	2.707215000	3.728657000
coord_9			
C	3.152631000	-1.052985000	0.140550000
C	3.130682000	0.371203000	0.014731000
C	1.977658000	1.080428000	-0.188865000
C	0.773275000	-1.007351000	-0.230781000
C	1.906996000	-1.730297000	-0.043952000
C	4.466625000	-1.561764000	0.336317000
C	5.427923000	-0.593577000	0.360955000
N	0.746658000	0.389514000	-0.174486000
H	-0.172458000	-1.483064000	-0.389539000
H	1.853308000	-2.802211000	-0.061620000
H	4.691025000	-2.604990000	0.450566000
H	6.481128000	-0.719316000	0.498656000
S	2.001310000	2.826998000	-0.511927000
S	4.769772000	1.027296000	0.140376000
C	-0.545302000	1.066002000	-0.021307000
O	-1.364711000	0.857428000	-1.176955000
C	-1.355697000	0.583584000	1.158819000
H	-0.417840000	2.143097000	0.080787000
C	-2.735937000	0.844081000	-0.754190000
C	-2.726044000	1.027206000	0.753238000
H	-1.026779000	1.016566000	2.106593000
H	-1.337275000	-0.503289000	1.268548000
H	-3.233652000	1.701117000	-1.213026000
H	-2.835377000	2.089076000	0.986791000
C	-3.419422000	-0.422751000	-1.264666000
H	-4.488621000	-0.400101000	-1.040028000
H	-3.294901000	-0.513808000	-2.346344000
O	-2.872993000	-1.596596000	-0.677364000
H	-2.829496000	-1.430525000	0.279016000
O	-3.753855000	0.311757000	1.426123000
H	-3.533946000	0.338559000	2.372020000
O	3.699026000	5.555471000	-1.778933000
H	3.540989000	4.860794000	-2.401896000
H	4.613218000	5.514578000	-1.537654000
O	4.884278000	2.240802000	3.692486000
H	4.935198000	1.897193000	2.811295000
H	4.059385000	2.704087000	3.730627000
coord_10			
C	3.156471000	-1.046750000	0.153865000

C	3.134334000	0.371931000	0.025260000
C	1.980005000	1.082367000	-0.181744000
C	0.777179000	-1.008731000	-0.225075000
C	1.906925000	-1.728472000	-0.038877000
C	4.469536000	-1.557346000	0.349476000
C	5.433404000	-0.591214000	0.371320000
N	0.746420000	0.391170000	-0.155900000
H	-0.168150000	-1.483811000	-0.389513000
H	1.857175000	-2.800640000	-0.063653000
H	4.692161000	-2.600921000	0.464933000
H	6.486637000	-0.715908000	0.508755000
S	2.012389000	2.825155000	-0.525371000
S	4.772619000	1.027245000	0.148301000
C	-0.542797000	1.068818000	0.007986000
O	-1.363435000	0.877362000	-1.150781000
C	-1.352963000	0.571578000	1.182665000
H	-0.409444000	2.144937000	0.125324000
C	-2.734362000	0.856813000	-0.726662000
C	-2.722951000	1.022533000	0.783396000
H	-1.022834000	0.991710000	2.136559000
H	-1.335667000	-0.517425000	1.277874000
H	-3.234149000	1.718559000	-1.175409000
H	-2.830215000	2.082332000	1.029488000
C	-3.416889000	-0.405708000	-1.250804000
H	-4.485944000	-0.386671000	-1.024774000
H	-3.293410000	-0.484603000	-2.334032000
O	-2.868886000	-1.586135000	-0.676934000
H	-2.825603000	-1.431037000	0.281765000
O	-3.751334000	0.300610000	1.448845000
H	-3.530161000	0.315301000	2.395298000
O	3.680747000	5.540776000	-1.749229000
H	3.565457000	4.896719000	-2.434574000
H	4.600388000	5.510892000	-1.524142000
O	4.894056000	2.244604000	3.705794000
H	4.942331000	1.885598000	2.829392000
H	4.063591000	2.699164000	3.740387000

S₁(¹nπ*) minimum to ¹nπ*/³ππ*

coord_1

C	3.168010900	-1.042290300	0.103688000
C	3.135126900	0.388565100	0.008919000
C	1.982508600	1.093285300	-0.186874100
C	0.785599200	-1.006763300	-0.250452100

C	1.918243500	-1.722202500	-0.065151000
C	4.475254300	-1.549645400	0.295311100
C	5.440760500	-0.575928200	0.351958100
N	0.757405200	0.394479100	-0.244975100
H	-0.159306000	-1.487760400	-0.400968100
H	1.866131500	-2.794467800	-0.069424000
H	4.699534300	-2.594860700	0.388321100
H	6.493232800	-0.700630200	0.494209100
S	2.016687600	2.860941800	-0.371244100
S	4.774636300	1.045681300	0.166021000
C	-0.545491200	1.062583300	-0.145435000
O	-1.356002400	0.768778200	-1.289194400
C	-1.355847400	0.643970200	1.059857300
H	-0.438018100	2.146365600	-0.116825000
C	-2.729345800	0.776633200	-0.873476200
C	-2.730019800	1.046432300	0.621926200
H	-1.035300300	1.136864300	1.981846600
H	-1.325305400	-0.434989100	1.234662300
H	-3.225279900	1.605742400	-1.383562400
H	-2.854292800	2.119206600	0.792237200
C	-3.403958000	-0.520232100	-1.315883400
H	-4.475674300	-0.487387100	-1.105270300
H	-3.265736900	-0.675123200	-2.389169700
O	-2.860547800	-1.655932500	-0.653993200
H	-2.833340800	-1.435895400	0.292534100
O	-3.753941100	0.359569100	1.330707400
H	-3.556522000	0.470104100	2.276088600
O	3.738933000	5.560077600	-1.919442500
H	3.522234000	4.773062300	-2.406992700
H	4.630857300	5.434900500	-1.624613500
O	4.875585400	2.229662600	3.692187000
H	4.916939400	1.827126500	2.834401800
H	4.044707100	2.684184800	3.711690000
coord_2			
C	3.168244000	-1.015187000	0.105770000
C	3.123691000	0.412491000	-0.001336000
C	1.964188000	1.106508000	-0.193067000
C	0.785615000	-1.001304000	-0.231409000
C	1.921941000	-1.706277000	-0.050514000
C	4.479937000	-1.511236000	0.291760000
C	5.438175000	-0.530545000	0.332119000
N	0.743976000	0.399208000	-0.227780000

H	-0.157370000	-1.488912000	-0.375187000
H	1.878691000	-2.779221000	-0.048213000
H	4.710234000	-2.554821000	0.392060000
H	6.492753000	-0.645151000	0.467917000
S	1.980542000	2.875445000	-0.395361000
S	4.757725000	1.082852000	0.137650000
C	-0.562433000	1.057046000	-0.115680000
O	-1.373919000	0.769741000	-1.260143000
C	-1.366894000	0.620684000	1.087324000
H	-0.462509000	2.141108000	-0.073941000
C	-2.746012000	0.773313000	-0.841340000
C	-2.742523000	1.025172000	0.657606000
H	-1.046166000	1.104208000	2.014208000
H	-1.334271000	-0.459948000	1.250167000
H	-3.242826000	1.608811000	-1.340029000
H	-2.867147000	2.095516000	0.842019000
C	-3.422306000	-0.517593000	-1.298046000
H	-4.492530000	-0.488682000	-1.079867000
H	-3.291725000	-0.656829000	-2.374574000
O	-2.873322000	-1.661763000	-0.655360000
H	-2.832375000	-1.451462000	0.292884000
O	-3.761734000	0.326672000	1.361491000
H	-3.551227000	0.410563000	2.306698000
O	3.780081000	5.507642000	-1.864412000
H	3.603321000	4.735290000	-2.384358000
H	4.657782000	5.376736000	-1.531815000
O	4.879614000	2.197941000	3.689721000
H	4.913439000	1.817101000	2.824466000
H	4.050860000	2.652694000	3.726350000

coord_3

C	3.168477000	-0.988083000	0.107851000
C	3.112255000	0.436418000	-0.011591000
C	1.945867000	1.119730000	-0.199260000
C	0.785631000	-0.995845000	-0.212366000
C	1.925637000	-1.690353000	-0.035877000
C	4.484620000	-1.472827000	0.288210000
C	5.435589000	-0.485162000	0.312279000
N	0.730546000	0.403937000	-0.210584000
H	-0.155013000	-1.490674000	-0.348929000
H	1.891259000	-2.763650000	-0.027460000
H	4.723315000	-2.513882000	0.396568000
H	6.492035000	-0.590452000	0.441759000

S	1.944397000	2.889948000	-0.419477000
S	4.740813000	1.120024000	0.109279000
C	-0.576926000	1.052416000	-0.061190000
O	-1.409217000	0.779645000	-1.194011000
C	-1.356640000	0.592440000	1.149548000
H	-0.480078000	2.136074000	-0.002823000
C	-2.773340000	0.773239000	-0.748665000
C	-2.742515000	0.996893000	0.754395000
H	-1.020514000	1.061426000	2.078327000
H	-1.316544000	-0.490752000	1.293555000
H	-3.280989000	1.616898000	-1.222201000
H	-2.870952000	2.062645000	0.961912000
C	-3.456678000	-0.510303000	-1.214979000
H	-4.521857000	-0.488660000	-0.971525000
H	-3.350466000	-0.627702000	-2.296557000
O	-2.889144000	-1.665092000	-0.608254000
H	-2.828252000	-1.474170000	0.343102000
O	-3.744245000	0.278899000	1.463893000
H	-3.516688000	0.345397000	2.406598000
O	3.821230000	5.455207000	-1.809381000
H	3.685242000	4.697760000	-2.362462000
H	4.682863000	5.318741000	-1.439135000
O	4.883644000	2.166219000	3.687254000
H	4.910023000	1.805934000	2.811756000
H	4.057013000	2.621204000	3.741011000
coord_4			
C	3.168710000	-0.960980000	0.109933000
C	3.100819000	0.460344000	-0.021846000
C	1.927546000	1.132953000	-0.205453000
C	0.785647000	-0.990386000	-0.193323000
C	1.929334000	-1.674428000	-0.021240000
C	4.489303000	-1.434418000	0.284659000
C	5.433003000	-0.439778000	0.292440000
N	0.717116000	0.408666000	-0.193389000
H	-0.151716000	-1.493765000	-0.322396000
H	1.903863000	-2.747978000	-0.006476000
H	4.736434000	-2.472756000	0.400467000
H	6.491165000	-0.536028000	0.414766000
S	1.908252000	2.904452000	-0.443593000
S	4.723901000	1.157195000	0.080907000
C	-0.595831000	1.050199000	-0.068195000
O	-1.404801000	0.774406000	-1.216734000

C	-1.395871000	0.587085000	1.127489000
H	-0.506266000	2.134382000	-0.007384000
C	-2.776883000	0.762576000	-0.797004000
C	-2.773981000	0.990845000	0.705450000
H	-1.077006000	1.057738000	2.061538000
H	-1.356546000	-0.496122000	1.271428000
H	-3.280238000	1.602390000	-1.281473000
H	-2.903436000	2.057739000	0.906241000
C	-3.444313000	-0.525435000	-1.273810000
H	-4.514530000	-0.508764000	-1.053809000
H	-3.313670000	-0.645448000	-2.352514000
O	-2.885278000	-1.675355000	-0.650758000
H	-2.845256000	-1.479289000	0.300575000
O	-3.790354000	0.277038000	1.397983000
H	-3.581536000	0.347614000	2.344745000
O	3.862378000	5.402771000	-1.754351000
H	3.768367000	4.663084000	-2.339279000
H	4.706127000	5.260956000	-1.346807000
O	4.887673000	2.134498000	3.684788000
H	4.906536000	1.795317000	2.800075000
H	4.060973000	2.590924000	3.755860000
coord_5			
C	3.168943000	-0.933876000	0.112015000
C	3.089383000	0.484270000	-0.032101000
C	1.909225000	1.146175000	-0.211646000
C	0.785663000	-0.984928000	-0.174281000
C	1.933031000	-1.658503000	-0.006603000
C	4.493985000	-1.396009000	0.281109000
C	5.430417000	-0.394395000	0.272600000
N	0.703686000	0.413396000	-0.176193000
H	-0.149062000	-1.495421000	-0.295612000
H	1.916757000	-2.732134000	0.014256000
H	4.749763000	-2.431422000	0.404722000
H	6.490126000	-0.481550000	0.388226000
S	1.872107000	2.918955000	-0.467710000
S	4.706990000	1.194366000	0.052536000
C	-0.610535000	1.045253000	-0.022091000
O	-1.434863000	0.780572000	-1.162445000
C	-1.392629000	0.565315000	1.179516000
H	-0.522661000	2.128464000	0.052063000
C	-2.800959000	0.759088000	-0.723445000
C	-2.777939000	0.969289000	0.781561000

H	-1.064030000	1.025675000	2.115362000
H	-1.347610000	-0.519174000	1.310939000
H	-3.314253000	1.602512000	-1.191163000
H	-2.909263000	2.033118000	0.997650000
C	-3.471771000	-0.525772000	-1.204435000
H	-4.537900000	-0.516198000	-0.964379000
H	-3.360452000	-0.631538000	-2.286703000
O	-2.896500000	-1.681581000	-0.607618000
H	-2.844152000	-1.500924000	0.346166000
O	-3.781854000	0.242922000	1.479191000
H	-3.557741000	0.298123000	2.423377000
O	3.903526000	5.350335000	-1.699320000
H	3.852295000	4.631198000	-2.314408000
H	4.727639000	5.203417000	-1.255058000
O	4.891702000	2.102776000	3.682322000
H	4.902997000	1.785421000	2.790152000
H	4.066870000	2.559579000	3.770593000
coord_6			
C	3.169176000	-0.906773000	0.114097000
C	3.077948000	0.508196000	-0.042356000
C	1.890904000	1.159398000	-0.217839000
C	0.785679000	-0.979469000	-0.155238000
C	1.936728000	-1.642578000	0.008034000
C	4.498668000	-1.357600000	0.277558000
C	5.427831000	-0.349011000	0.252761000
N	0.690257000	0.418125000	-0.158998000
H	-0.145785000	-1.497800000	-0.269062000
H	1.929786000	-2.716177000	0.034928000
H	4.763155000	-2.389891000	0.408646000
H	6.488940000	-0.427332000	0.361375000
S	1.835961000	2.933458000	-0.491826000
S	4.690078000	1.231538000	0.024165000
C	-0.627811000	1.043209000	-0.008446000
O	-1.445236000	0.781165000	-1.154237000
C	-1.414554000	0.555151000	1.186438000
H	-0.544501000	2.126384000	0.072695000
C	-2.813641000	0.752129000	-0.722194000
C	-2.799036000	0.957440000	0.783616000
H	-1.091112000	1.011186000	2.126153000
H	-1.367665000	-0.529835000	1.311995000
H	-3.328601000	1.594739000	-1.189906000
H	-2.935454000	2.019840000	1.003306000

C	-3.474885000	-0.535169000	-1.209619000
H	-4.542390000	-0.532486000	-0.975785000
H	-3.357029000	-0.637002000	-2.291604000
O	-2.896795000	-1.689480000	-0.611804000
H	-2.849752000	-1.510601000	0.342654000
O	-3.803752000	0.225449000	1.473737000
H	-3.583668000	0.278989000	2.419066000
O	3.944675000	5.297900000	-1.644290000
H	3.936587000	4.601948000	-2.287486000
H	4.747496000	5.146156000	-1.164114000
O	4.895731000	2.071054000	3.679856000
H	4.899458000	1.775501000	2.780165000
H	4.073043000	2.528081000	3.785303000
coord_7			
C	3.169409000	-0.879669000	0.116178000
C	3.066512000	0.532122000	-0.052610000
C	1.872583000	1.172620000	-0.224032000
C	0.785695000	-0.974010000	-0.136195000
C	1.940425000	-1.626653000	0.022671000
C	4.503351000	-1.319191000	0.274008000
C	5.425245000	-0.303628000	0.232922000
N	0.676827000	0.422854000	-0.141802000
H	-0.142120000	-1.500495000	-0.242736000
H	1.943055000	-2.700083000	0.055392000
H	4.776668000	-2.348155000	0.412744000
H	6.487608000	-0.373334000	0.334486000
S	1.799816000	2.947962000	-0.515942000
S	4.673166000	1.268709000	-0.004206000
C	-0.644296000	1.040815000	-0.003055000
O	-1.445620000	0.780915000	-1.160091000
C	-1.442606000	0.543941000	1.180169000
H	-0.565685000	2.123893000	0.084199000
C	-2.818490000	0.745511000	-0.744801000
C	-2.822285000	0.946522000	0.761750000
H	-1.130518000	0.996341000	2.125517000
H	-1.394706000	-0.541616000	1.300919000
H	-3.330702000	1.587535000	-1.216187000
H	-2.960510000	2.008583000	0.982298000
C	-3.469146000	-0.542402000	-1.244737000
H	-4.539564000	-0.541681000	-1.025571000
H	-3.336179000	-0.642181000	-2.325230000
O	-2.897509000	-1.696859000	-0.641258000

H	-2.861601000	-1.518457000	0.313662000
O	-3.835480000	0.212859000	1.437305000
H	-3.626501000	0.262266000	2.385240000
O	3.985823000	5.245464000	-1.589259000
H	4.020785000	4.575093000	-2.258211000
H	4.765821000	5.089204000	-1.074185000
O	4.899760000	2.039332000	3.677389000
H	4.895923000	1.765761000	2.770773000
H	4.079490000	2.496431000	3.799971000
coord_8			
C	3.169642000	-0.852566000	0.118260000
C	3.055076000	0.556049000	-0.062865000
C	1.854262000	1.185842000	-0.230225000
C	0.785710000	-0.968551000	-0.117152000
C	1.944122000	-1.610728000	0.037308000
C	4.508034000	-1.280782000	0.270457000
C	5.422660000	-0.258245000	0.213082000
N	0.663397000	0.427583000	-0.124607000
H	-0.138576000	-1.502632000	-0.216413000
H	1.956469000	-2.683857000	0.075642000
H	4.790317000	-2.306220000	0.416957000
H	6.486112000	-0.319470000	0.307827000
S	1.763671000	2.962465000	-0.540059000
S	4.656255000	1.305880000	-0.032578000
C	-0.661588000	1.038833000	0.012181000
O	-1.454639000	0.788096000	-1.152613000
C	-1.466534000	0.530410000	1.186046000
H	-0.586724000	2.121288000	0.110874000
C	-2.830213000	0.742691000	-0.746170000
C	-2.844502000	0.932089000	0.761689000
H	-1.162770000	0.976593000	2.137087000
H	-1.417609000	-0.555782000	1.298805000
H	-3.344721000	1.584976000	-1.214862000
H	-2.987064000	1.991783000	0.989935000
C	-3.470515000	-0.545628000	-1.258051000
H	-4.542526000	-0.552608000	-1.046083000
H	-3.329894000	-0.638547000	-2.338060000
O	-2.895064000	-1.699704000	-0.657599000
H	-2.868552000	-1.527375000	0.298859000
O	-3.859509000	0.189855000	1.425176000
H	-3.656348000	0.232162000	2.374737000
O	4.026971000	5.193029000	-1.534228000

H	4.104439000	4.550319000	-2.226355000
H	4.782769000	5.032581000	-0.985463000
O	4.903789000	2.007611000	3.674923000
H	4.892404000	1.756158000	2.761988000
H	4.086208000	2.464629000	3.814580000
coord_9			
C	3.169875000	-0.825462000	0.120342000
C	3.043640000	0.579975000	-0.073120000
C	1.835941000	1.199065000	-0.236418000
C	0.785726000	-0.963092000	-0.098109000
C	1.947819000	-1.594803000	0.051945000
C	4.512716000	-1.242373000	0.266906000
C	5.420074000	-0.212861000	0.193243000
N	0.649968000	0.432312000	-0.107412000
H	-0.135302000	-1.504482000	-0.190334000
H	1.970539000	-2.667984000	0.095865000
H	4.804065000	-2.264313000	0.420987000
H	6.484511000	-0.266068000	0.280873000
S	1.727526000	2.976968000	-0.564175000
S	4.639343000	1.343051000	-0.060949000
C	-0.676788000	1.036219000	0.032193000
O	-1.466690000	0.790527000	-1.135516000
C	-1.480509000	0.515971000	1.201231000
H	-0.605192000	2.118168000	0.138721000
C	-2.842490000	0.737778000	-0.730967000
C	-2.858670000	0.917694000	0.778172000
H	-1.178223000	0.954211000	2.156514000
H	-1.428432000	-0.570936000	1.304242000
H	-3.359099000	1.581693000	-1.194193000
H	-3.003506000	1.975902000	1.011773000
C	-3.477429000	-0.548481000	-1.253996000
H	-4.549657000	-0.561005000	-1.043745000
H	-3.334793000	-0.631609000	-2.334613000
O	-2.898413000	-1.705519000	-0.662695000
H	-2.872753000	-1.541079000	0.295016000
O	-3.872312000	0.170182000	1.437527000
H	-3.667522000	0.206522000	2.387064000
O	4.068120000	5.140593000	-1.479198000
H	4.187130000	4.527258000	-2.191780000
H	4.798510000	4.976306000	-0.898116000
O	4.907819000	1.975889000	3.672457000
H	4.888940000	1.746921000	2.754914000

H	4.093932000	2.432260000	3.828973000
coord_10			
C	3.170108300	-0.798358900	0.122423200
C	3.032204300	0.603901100	-0.083375200
C	1.817620600	1.212287300	-0.242611200
C	0.785742300	-0.957632900	-0.079066100
C	1.951516200	-1.578878000	0.066581800
C	4.517399300	-1.203964200	0.263356000
C	5.417487900	-0.167478100	0.173403400
N	0.636537800	0.437041100	-0.090216200
H	-0.129393400	-1.509819600	-0.163869700
H	1.980585000	-2.650302200	0.117062400
H	4.817099100	-2.222068300	0.425680100
H	6.483546200	-0.210592900	0.252549800
S	1.691380400	2.991471500	-0.588291600
S	4.622431500	1.380222600	-0.089320100
C	-0.691349000	1.033230300	0.058512500
O	-1.477348000	0.803962900	-1.114680300
C	-1.496446900	0.494209000	1.218453300
H	-0.619988500	2.113163400	0.182109000
C	-2.853486700	0.738150400	-0.713826000
C	-2.873977400	0.900004300	0.797277300
H	-1.197459900	0.919424600	2.180477100
H	-1.443250200	-0.593765600	1.307259500
H	-3.373812200	1.584265900	-1.168823900
H	-3.019408600	1.955209300	1.043613700
C	-3.479492300	-0.546392200	-1.252149400
H	-4.552405500	-0.566178300	-1.046381800
H	-3.332157700	-0.618094700	-2.332987700
O	-2.898169500	-1.706802300	-0.669665800
H	-2.878028600	-1.552019000	0.289966600
O	-3.889384300	0.144110800	1.444326200
H	-3.689848700	0.170931400	2.395285300
O	4.109267900	5.088157800	-1.424167300
H	4.268537500	4.505314200	-2.154675800
H	4.813527800	4.920317300	-0.812029400
O	4.911847700	1.944167100	3.669990800
H	4.885439800	1.736894900	2.744978000
H	4.100085100	2.400769400	3.843632900
$^1n\pi^*/^3\pi\pi^*$ to $T_1(^3\pi\pi^*)$ minimum			
coord_1			
C	3.210278900	-0.806598200	0.153924000

C	3.070894900	0.596091200	-0.047913000
C	1.855670500	1.203640300	-0.205448100
C	0.826085200	-0.967823300	-0.048052000
C	1.992513600	-1.588244400	0.095858000
C	4.557996300	-1.211175300	0.293731100
C	5.456989500	-0.173488000	0.206722100
N	0.675406200	0.426718100	-0.055263000
H	-0.088465000	-1.520735400	-0.134430000
H	2.022714600	-2.659775700	0.143311000
H	4.858770400	-2.229416600	0.453182100
H	6.523091800	-0.215699100	0.285763100
S	1.727553500	2.983659800	-0.546101200
S	4.660300300	1.374107400	-0.051639000
C	-0.653112200	1.021080300	0.095129000
O	-1.438853400	0.794298200	-1.078719300
C	-1.457654400	0.477932100	1.253529400
H	-0.582895200	2.100734600	0.221778100
C	-2.814926800	0.725898200	-0.678074200
C	-2.835607800	0.883459200	0.833480200
H	-1.159129300	0.900743300	2.216755600
H	-1.403308400	-0.610232200	1.339261400
H	-3.336140900	1.572745400	-1.130687300
H	-2.982157800	1.937809500	1.082795300
C	-3.439567000	-0.557779200	-1.220035300
H	-4.512461300	-0.579281200	-1.014341300
H	-3.292142900	-0.626271200	-2.301069600
O	-2.857024800	-1.719215500	-0.640824200
H	-2.837059800	-1.567123400	0.319242100
O	-3.850223100	0.124667000	1.478374400
H	-3.650728000	0.149011000	2.429408700
O	4.143233200	5.085255400	-1.376010400
H	4.303128200	4.504647300	-2.108160600
H	4.847662400	4.916430400	-0.764338200
O	4.949072400	1.927731500	3.709255000
H	4.922895400	1.723046500	2.783659800
H	4.136825200	2.382982700	3.884174100
coord_2			
C	3.206287000	-0.834176000	0.159858000
C	3.078269000	0.572855000	-0.038939000
C	1.868461000	1.189714000	-0.201535000
C	0.821897000	-0.974396000	-0.055767000
C	1.986421000	-1.604499000	0.092340000

C	4.550384000	-1.248139000	0.305429000
C	5.455564000	-0.216896000	0.226677000
N	0.683136000	0.420666000	-0.058079000
H	-0.095648000	-1.521081000	-0.147108000
H	2.010102000	-2.676680000	0.136154000
H	4.843010000	-2.268993000	0.462600000
H	6.520510000	-0.269624000	0.311524000
S	1.756186000	2.961665000	-0.542883000
S	4.673140000	1.338224000	-0.032780000
C	-0.643584000	1.024976000	0.086614000
O	-1.432577000	0.797341000	-1.085647000
C	-1.450499000	0.492124000	1.247791000
H	-0.568728000	2.105389000	0.207602000
C	-2.809135000	0.735086000	-0.683519000
C	-2.828653000	0.897139000	0.827647000
H	-1.149949000	0.921085000	2.207585000
H	-1.397787000	-0.595662000	1.340375000
H	-3.328913000	1.582072000	-1.137971000
H	-2.975885000	1.952007000	1.074542000
C	-3.437988000	-0.548373000	-1.221100000
H	-4.510675000	-0.567150000	-1.013920000
H	-3.292244000	-0.620141000	-2.302126000
O	-2.856952000	-1.709326000	-0.639354000
H	-2.835264000	-1.554365000	0.320132000
O	-3.842422000	0.139915000	1.475961000
H	-3.642962000	0.168947000	2.426915000
O	4.103643000	5.141824000	-1.426270000
H	4.287617000	4.510201000	-2.107818000
H	4.780167000	5.020595000	-0.774411000
O	4.952275000	1.966078000	3.703355000
H	4.928184000	1.743804000	2.783125000
H	4.139559000	2.423552000	3.867732000
coord_3			
C	3.202296000	-0.861753000	0.165792000
C	3.085643000	0.549618000	-0.029964000
C	1.881252000	1.175787000	-0.197622000
C	0.817709000	-0.980970000	-0.063481000
C	1.980328000	-1.620753000	0.088821000
C	4.542772000	-1.285103000	0.317126000
C	5.454138000	-0.260305000	0.246633000
N	0.690867000	0.414613000	-0.060895000
H	-0.103021000	-1.520965000	-0.159933000

H	1.995222000	-2.693231000	0.129128000
H	4.827882000	-2.308312000	0.472193000
H	6.518188000	-0.321066000	0.336757000
S	1.784818000	2.939670000	-0.539664000
S	4.685979000	1.302341000	-0.013922000
C	-0.632073000	1.025605000	0.082374000
O	-1.421479000	0.794050000	-1.088627000
C	-1.440729000	0.502469000	1.246992000
H	-0.552323000	2.106233000	0.197212000
C	-2.797823000	0.740629000	-0.686739000
C	-2.816759000	0.911923000	0.823447000
H	-1.138632000	0.935098000	2.204923000
H	-1.392539000	-0.585111000	1.345501000
H	-3.312773000	1.587326000	-1.146759000
H	-2.958121000	1.969308000	1.063761000
C	-3.432901000	-0.542810000	-1.217122000
H	-4.505479000	-0.554773000	-1.009086000
H	-3.288245000	-0.621684000	-2.297845000
O	-2.857484000	-1.703340000	-0.629196000
H	-2.834453000	-1.542819000	0.329334000
O	-3.835674000	0.163671000	1.474061000
H	-3.636194000	0.192989000	2.424914000
O	4.064053000	5.198392000	-1.476530000
H	4.272252000	4.516918000	-2.100667000
H	4.708412000	5.127265000	-0.785846000
O	4.955477000	2.004424000	3.697455000
H	4.933451000	1.764313000	2.781665000
H	4.142041000	2.464263000	3.851336000
coord_4			
C	3.198304000	-0.889331000	0.171726000
C	3.093017000	0.526381000	-0.020990000
C	1.894042000	1.161861000	-0.193709000
C	0.813520000	-0.987543000	-0.071196000
C	1.974236000	-1.637007000	0.085303000
C	4.535160000	-1.322066000	0.328824000
C	5.452712000	-0.303713000	0.266588000
N	0.698597000	0.408560000	-0.063711000
H	-0.110343000	-1.520783000	-0.172772000
H	1.980372000	-2.709712000	0.122095000
H	4.812741000	-2.347584000	0.481761000
H	6.515795000	-0.372446000	0.362000000
S	1.813451000	2.917674000	-0.536445000

S	4.698818000	1.266458000	0.004937000
C	-0.620038000	1.028791000	0.077947000
O	-1.411210000	0.800592000	-1.092853000
C	-1.430549000	0.509895000	1.242693000
H	-0.533557000	2.109000000	0.192486000
C	-2.787521000	0.750158000	-0.690111000
C	-2.805034000	0.923208000	0.819457000
H	-1.126363000	0.942507000	2.199819000
H	-1.386429000	-0.577725000	1.341928000
H	-3.300311000	1.598078000	-1.150391000
H	-2.942749000	1.981409000	1.057680000
C	-3.426860000	-0.532044000	-1.218725000
H	-4.499816000	-0.539486000	-1.012466000
H	-3.281013000	-0.612414000	-2.299133000
O	-2.857264000	-1.694798000	-0.628838000
H	-2.832007000	-1.533742000	0.329610000
O	-3.825045000	0.178877000	1.472785000
H	-3.627147000	0.215019000	2.423780000
O	4.024463000	5.254961000	-1.526790000
H	4.256282000	4.526784000	-2.086540000
H	4.631868000	5.235898000	-0.800155000
O	4.958679000	2.042771000	3.691554000
H	4.938731000	1.784881000	2.780564000
H	4.144628000	2.504917000	3.834910000
coord_5			
C	3.194313000	-0.916909000	0.177660000
C	3.100391000	0.503145000	-0.012015000
C	1.906833000	1.147934000	-0.189796000
C	0.809332000	-0.994116000	-0.078910000
C	1.968143000	-1.653262000	0.081784000
C	4.527548000	-1.359030000	0.340521000
C	5.451287000	-0.347121000	0.286543000
N	0.706327000	0.402508000	-0.066526000
H	-0.117605000	-1.520611000	-0.185594000
H	1.965549000	-2.726129000	0.115054000
H	4.797584000	-2.386808000	0.491333000
H	6.513331000	-0.423837000	0.387229000
S	1.842083000	2.895679000	-0.533227000
S	4.711658000	1.230575000	0.023796000
C	-0.608809000	1.031016000	0.074683000
O	-1.401270000	0.807240000	-1.096284000
C	-1.422543000	0.517214000	1.239566000

H	-0.516008000	2.110912000	0.188759000
C	-2.777884000	0.761024000	-0.693919000
C	-2.795209000	0.935440000	0.815362000
H	-1.117768000	0.950021000	2.196406000
H	-1.382562000	-0.570497000	1.340506000
H	-3.288451000	1.609927000	-1.154908000
H	-2.928754000	1.994360000	1.052795000
C	-3.420738000	-0.519914000	-1.221545000
H	-4.493891000	-0.523952000	-1.015873000
H	-3.274534000	-0.602104000	-2.301729000
O	-2.855149000	-1.683674000	-0.629986000
H	-2.830596000	-1.521765000	0.328326000
O	-3.818522000	0.195532000	1.468577000
H	-3.620644000	0.231092000	2.419647000
O	3.984873000	5.311529000	-1.577050000
H	4.239046000	4.541301000	-2.066383000
H	4.550886000	5.345635000	-0.818256000
O	4.961881000	2.081117000	3.685654000
H	4.944020000	1.805527000	2.779817000
H	4.147321000	2.545512000	3.818462000
coord_6			
C	3.190321000	-0.944486000	0.183594000
C	3.107765000	0.479908000	-0.003041000
C	1.919623000	1.134008000	-0.185883000
C	0.805144000	-1.000689000	-0.086625000
C	1.962050000	-1.669516000	0.078265000
C	4.519936000	-1.395993000	0.352219000
C	5.449861000	-0.390529000	0.306499000
N	0.714057000	0.396456000	-0.069342000
H	-0.124818000	-1.520403000	-0.198392000
H	1.950752000	-2.742484000	0.108006000
H	4.782385000	-2.425989000	0.500898000
H	6.510806000	-0.475207000	0.412446000
S	1.870715000	2.873684000	-0.530008000
S	4.724497000	1.194691000	0.042654000
C	-0.597718000	1.033159000	0.072240000
O	-1.391588000	0.814053000	-1.099028000
C	-1.415044000	0.524208000	1.237386000
H	-0.498388000	2.112624000	0.185925000
C	-2.768664000	0.771505000	-0.697567000
C	-2.786092000	0.947461000	0.811759000
H	-1.109703000	0.956930000	2.194069000

H	-1.378988000	-0.563450000	1.341245000
H	-3.277128000	1.620543000	-1.160533000
H	-2.916439000	2.006802000	1.048802000
C	-3.415345000	-0.507809000	-1.224406000
H	-4.488302000	-0.508807000	-1.017577000
H	-3.270050000	-0.592225000	-2.304573000
O	-2.852632000	-1.671808000	-0.631553000
H	-2.830424000	-1.508072000	0.326383000
O	-3.812247000	0.212720000	1.466042000
H	-3.612325000	0.248821000	2.416665000
O	3.945283000	5.368098000	-1.627310000
H	4.219924000	4.561748000	-2.041646000
H	4.466083000	5.455503000	-0.840907000
O	4.965084000	2.119464000	3.679754000
H	4.949317000	1.826273000	2.779421000
H	4.150120000	2.586047000	3.801993000
coord_7			
C	3.186330000	-0.972064000	0.189528000
C	3.115139000	0.456672000	0.005933000
C	1.932414000	1.120081000	-0.181970000
C	0.800955000	-1.007262000	-0.094340000
C	1.955958000	-1.685771000	0.074747000
C	4.512324000	-1.432957000	0.363916000
C	5.448436000	-0.433938000	0.326454000
N	0.721787000	0.390403000	-0.072158000
H	-0.131972000	-1.520173000	-0.211186000
H	1.935985000	-2.758776000	0.100955000
H	4.767190000	-2.465118000	0.510449000
H	6.508212000	-0.526578000	0.437659000
S	1.899347000	2.851689000	-0.526789000
S	4.737337000	1.158808000	0.061513000
C	-0.585607000	1.035484000	0.069337000
O	-1.381706000	0.819845000	-1.101160000
C	-1.403956000	0.531103000	1.235554000
H	-0.479680000	2.114499000	0.181690000
C	-2.758352000	0.782363000	-0.698284000
C	-2.773659000	0.959352000	0.810708000
H	-1.094982000	0.963063000	2.191583000
H	-1.372359000	-0.556614000	1.339534000
H	-3.264046000	1.633425000	-1.160753000
H	-2.898684000	2.019404000	1.046914000
C	-3.410405000	-0.494909000	-1.224260000

H	-4.483508000	-0.490709000	-1.018532000
H	-3.264425000	-0.579831000	-2.304324000
O	-2.854520000	-1.662222000	-0.631016000
H	-2.827668000	-1.498379000	0.326909000
O	-3.803364000	0.229708000	1.465155000
H	-3.604932000	0.266540000	2.415957000
O	3.905693000	5.424666000	-1.677569000
H	4.198417000	4.589005000	-2.014147000
H	4.378304000	5.564506000	-0.868629000
O	4.968286000	2.157810000	3.673854000
H	4.954619000	1.847139000	2.779367000
H	4.153024000	2.626522000	3.785508000
coord_8			
C	3.182338000	-0.999641000	0.195462000
C	3.122513000	0.433435000	0.014908000
C	1.945205000	1.106155000	-0.178057000
C	0.796767000	-1.013835000	-0.102054000
C	1.949865000	-1.702025000	0.071228000
C	4.504712000	-1.469920000	0.375614000
C	5.447010000	-0.477346000	0.346409000
N	0.729518000	0.384350000	-0.074974000
H	-0.139065000	-1.519926000	-0.223963000
H	1.921247000	-2.775007000	0.093902000
H	4.751984000	-2.504197000	0.519996000
H	6.505550000	-0.577932000	0.462855000
S	1.927980000	2.829694000	-0.523571000
S	4.750176000	1.122925000	0.080372000
C	-0.573568000	1.037942000	0.066576000
O	-1.370920000	0.826388000	-1.103945000
C	-1.394582000	0.538127000	1.232660000
H	-0.461005000	2.116355000	0.179837000
C	-2.747776000	0.793147000	-0.701326000
C	-2.762332000	0.971772000	0.807404000
H	-1.083669000	0.970214000	2.187848000
H	-1.367724000	-0.549615000	1.338167000
H	-3.250149000	1.645491000	-1.164677000
H	-2.883018000	2.032909000	1.041470000
C	-3.404485000	-0.481900000	-1.227103000
H	-4.478033000	-0.474135000	-1.023081000
H	-3.257977000	-0.568453000	-2.306874000
O	-2.852707000	-1.650438000	-0.632639000
H	-2.826709000	-1.485834000	0.325109000

O	-3.794541000	0.246079000	1.462941000
H	-3.596203000	0.282577000	2.413892000
O	3.866103000	5.481234000	-1.727829000
H	4.174210000	4.623450000	-1.985857000
H	4.288540000	5.671712000	-0.901653000
O	4.971488000	2.196156000	3.667953000
H	4.959924000	1.868144000	2.779650000
H	4.156035000	2.666935000	3.769011000
coord_9			
C	3.178347000	-1.027219000	0.201396000
C	3.129887000	0.410199000	0.023882000
C	1.957995000	1.092228000	-0.174144000
C	0.792579000	-1.020408000	-0.109769000
C	1.943772000	-1.718279000	0.067710000
C	4.497100000	-1.506884000	0.387311000
C	5.445584000	-0.520754000	0.366365000
N	0.737248000	0.378298000	-0.077790000
H	-0.146102000	-1.519657000	-0.236731000
H	1.906535000	-2.791176000	0.086856000
H	4.736882000	-2.543200000	0.529530000
H	6.502823000	-0.629268000	0.488040000
S	1.956612000	2.807699000	-0.520352000
S	4.763016000	1.087042000	0.099230000
C	-0.562628000	1.040613000	0.059349000
O	-1.357557000	0.833412000	-1.113876000
C	-1.391213000	0.548442000	1.223989000
H	-0.443060000	2.118327000	0.171154000
C	-2.735906000	0.802143000	-0.716270000
C	-2.756395000	0.984640000	0.791792000
H	-1.083715000	0.983397000	2.179000000
H	-1.367739000	-0.538878000	1.334643000
H	-3.236551000	1.652929000	-1.184506000
H	-2.875828000	2.046554000	1.023045000
C	-3.391153000	-0.474677000	-1.239630000
H	-4.465372000	-0.464436000	-1.039953000
H	-3.239900000	-0.566584000	-2.318376000
O	-2.844493000	-1.641096000	-0.636405000
H	-2.823157000	-1.471338000	0.320591000
O	-3.793849000	0.263492000	1.444108000
H	-3.599357000	0.300265000	2.395751000
O	3.826513000	5.537803000	-1.778089000
H	4.147185000	4.664955000	-1.958667000

H	4.197835000	5.776333000	-0.939921000
O	4.974691000	2.234503000	3.662053000
H	4.965229000	1.889308000	2.780260000
H	4.159152000	2.707286000	3.752508000
coord_10			
C	3.174355300	-1.054796600	0.207329700
C	3.137261500	0.386962200	0.032856600
C	1.970785800	1.078301900	-0.170230500
C	0.788390500	-1.026981100	-0.117483300
C	1.937679800	-1.734533700	0.064191300
C	4.489488300	-1.543847700	0.399008800
C	5.444158600	-0.564162400	0.386319900
N	0.744977900	0.372245400	-0.080605500
H	-0.153163200	-1.519310600	-0.249173400
H	1.892078100	-2.807277200	0.080628900
H	4.722033900	-2.582130500	0.538808300
H	6.500023400	-0.680605500	0.513299500
S	1.985244400	2.785703600	-0.517133500
S	4.775855000	1.051158500	0.118089000
C	-0.551124600	1.042730900	0.055100400
O	-1.347180100	0.838356300	-1.118190400
C	-1.382954400	0.557391500	1.220353600
H	-0.424946500	2.119743700	0.165002600
C	-2.725782600	0.811712800	-0.721019600
C	-2.746502400	0.997436300	0.786552600
H	-1.074553500	0.993852300	2.174445100
H	-1.363398800	-0.529702800	1.334213300
H	-3.223950500	1.662912700	-1.191416100
H	-2.862863700	2.060179000	1.015480500
C	-3.384984400	-0.464287000	-1.242002400
H	-4.459253800	-0.449952800	-1.043120700
H	-3.233210600	-0.559168700	-2.320333500
O	-2.843039200	-1.631235500	-0.635682200
H	-2.821372300	-1.459305200	0.320930000
O	-3.786799300	0.280865300	1.439607400
H	-3.593197200	0.319082200	2.391338200
O	3.786923500	5.594371200	-1.828349100
H	4.117401800	4.713002700	-1.934186200
H	4.107166900	5.877756300	-0.983178400
O	4.977892800	2.272849300	3.656153000
H	4.970521600	1.910113000	2.779893200
H	4.162459900	2.747523800	3.735991900

T₂(³nπ*) minimum to ³nπ*/³ππ*

coord_1

C	3.221740900	-0.808990200	0.204430100
C	3.113421900	0.587094200	-0.038355000
C	1.906813500	1.211761300	-0.226081100
C	0.830162200	-0.938956300	-0.027452000
C	2.007273600	-1.576937400	0.139797000
C	4.569816300	-1.241635300	0.349764100
C	5.480717500	-0.233284100	0.232963100
N	0.705520200	0.468764100	-0.013726000
H	-0.091794000	-1.475311400	-0.126363000
H	2.028600600	-2.649344700	0.181429100
H	4.847699400	-2.262269600	0.531686100
H	6.545794800	-0.296667100	0.311845100
S	1.766319500	2.947419800	-0.604695200
S	4.722333300	1.327494400	-0.068464000
C	-0.608287200	1.089436300	0.159376000
O	-1.398754400	0.918012300	-1.021238300
C	-1.423850400	0.530180100	1.302531400
H	-0.511207100	2.162202600	0.322662100
C	-2.775156800	0.845536200	-0.623356200
C	-2.795919800	0.964284300	0.891388200
H	-1.121529300	0.926898300	2.275858600
H	-1.383630400	-0.560095200	1.364226400
H	-3.291707900	1.705832500	-1.055573300
H	-2.930720800	2.013612600	1.167662300
C	-3.405353000	-0.421058100	-1.198545300
H	-4.478988300	-0.441126100	-0.996703300
H	-3.254967900	-0.463751100	-2.280472600
O	-2.832308800	-1.600333400	-0.646499200
H	-2.812528800	-1.471213400	0.316828100
O	-3.820591100	0.200772100	1.514288400
H	-3.622925000	0.198681100	2.466089700
O	4.047073100	4.798969300	-1.092271300
H	4.295292200	4.425816200	-1.928017500
H	4.834617400	4.784014300	-0.562816200
O	4.914975400	2.011749600	3.697273000
H	4.934319400	1.745086500	2.787228800
H	4.064828100	2.413207700	3.816627100

coord_2

C	3.215991000	-0.836141000	0.204406000
C	3.115604000	0.565014000	-0.030827000

C	1.913463000	1.197099000	-0.220271000
C	0.825034000	-0.948553000	-0.037788000
C	1.999046000	-1.594275000	0.131076000
C	4.560400000	-1.275066000	0.354895000
C	5.476178000	-0.269913000	0.249630000
N	0.709436000	0.458225000	-0.021526000
H	-0.098159000	-1.482453000	-0.139875000
H	2.013906000	-2.666967000	0.170084000
H	4.831771000	-2.298445000	0.532526000
H	6.540320000	-0.341001000	0.333988000
S	1.790206000	2.929608000	-0.595408000
S	4.727823000	1.296927000	-0.048148000
C	-0.606628000	1.079650000	0.134167000
O	-1.396570000	0.876601000	-1.042297000
C	-1.419917000	0.539227000	1.287451000
H	-0.515317000	2.156679000	0.273167000
C	-2.773276000	0.810061000	-0.643408000
C	-2.794466000	0.957144000	0.868799000
H	-1.119006000	0.956115000	2.252523000
H	-1.374327000	-0.549705000	1.369552000
H	-3.290219000	1.662443000	-1.090581000
H	-2.935084000	2.010713000	1.125002000
C	-3.404344000	-0.466822000	-1.195150000
H	-4.477588000	-0.484125000	-0.990658000
H	-3.255447000	-0.529049000	-2.276357000
O	-2.830210000	-1.635516000	-0.622657000
H	-2.808215000	-1.487964000	0.337938000
O	-3.813914000	0.199511000	1.507467000
H	-3.619731000	0.223799000	2.459632000
O	4.017759000	4.887445000	-1.174586000
H	4.286919000	4.438094000	-1.963850000
H	4.769098000	4.906046000	-0.598006000
O	4.921547000	2.040990000	3.692258000
H	4.937912000	1.763628000	2.785977000
H	4.075263000	2.450596000	3.807214000
coord_3			
C	3.210240000	-0.863293000	0.204382000
C	3.117785000	0.542933000	-0.023299000
C	1.920111000	1.182437000	-0.214461000
C	0.819906000	-0.958150000	-0.048123000
C	1.990818000	-1.611612000	0.122356000
C	4.550984000	-1.308497000	0.360026000

C	5.471638000	-0.306542000	0.266296000
N	0.713353000	0.447686000	-0.029327000
H	-0.105685000	-1.486934000	-0.153948000
H	1.998014000	-2.684474000	0.158525000
H	4.817373000	-2.333901000	0.532995000
H	6.534905000	-0.383252000	0.355985000
S	1.814093000	2.911797000	-0.586121000
S	4.733312000	1.266360000	-0.027832000
C	-0.599233000	1.076390000	0.130422000
O	-1.390405000	0.885000000	-1.046980000
C	-1.416371000	0.536458000	1.281864000
H	-0.501450000	2.152283000	0.274229000
C	-2.767532000	0.825773000	-0.648555000
C	-2.787878000	0.966260000	0.864260000
H	-1.113536000	0.946927000	2.249154000
H	-1.378433000	-0.553073000	1.359744000
H	-3.279738000	1.682608000	-1.092820000
H	-2.921228000	2.019416000	1.125838000
C	-3.406195000	-0.445183000	-1.204784000
H	-4.479535000	-0.456572000	-1.000433000
H	-3.258352000	-0.504695000	-2.286199000
O	-2.838472000	-1.619005000	-0.636062000
H	-2.817559000	-1.475422000	0.325126000
O	-3.813486000	0.212541000	1.497740000
H	-3.615316000	0.222136000	2.449245000
O	3.988444000	4.975921000	-1.256901000
H	4.277817000	4.448044000	-1.988277000
H	4.699503000	5.029355000	-0.633329000
O	4.928118000	2.070230000	3.687242000
H	4.941505000	1.782170000	2.784725000
H	4.085512000	2.488077000	3.797824000

coord_4

C	3.204490000	-0.890444000	0.204359000
C	3.119967000	0.520853000	-0.015771000
C	1.926760000	1.167774000	-0.208652000
C	0.814778000	-0.967747000	-0.058458000
C	1.982590000	-1.628950000	0.113635000
C	4.541568000	-1.341928000	0.365156000
C	5.467098000	-0.343172000	0.282963000
N	0.717269000	0.437147000	-0.037127000
H	-0.113186000	-1.491377000	-0.168010000
H	1.982129000	-2.701940000	0.146942000

H	4.803121000	-2.369290000	0.533383000
H	6.529445000	-0.425514000	0.377975000
S	1.837979000	2.893985000	-0.576833000
S	4.738801000	1.235793000	-0.007517000
C	-0.592830000	1.072158000	0.119835000
O	-1.384974000	0.880048000	-1.057123000
C	-1.412069000	0.538709000	1.272764000
H	-0.490853000	2.148281000	0.259487000
C	-2.762216000	0.825061000	-0.658438000
C	-2.782319000	0.970075000	0.853906000
H	-1.108933000	0.952300000	2.238590000
H	-1.377079000	-0.550702000	1.355106000
H	-3.272006000	1.682022000	-1.105197000
H	-2.912847000	2.024328000	1.112261000
C	-3.404313000	-0.446208000	-1.210383000
H	-4.477751000	-0.453965000	-1.006440000
H	-3.256409000	-0.509627000	-2.291603000
O	-2.840578000	-1.619922000	-0.637495000
H	-2.818688000	-1.473236000	0.323364000
O	-3.809273000	0.221097000	1.490739000
H	-3.610745000	0.234878000	2.442123000
O	3.959130000	5.064396000	-1.339215000
H	4.266530000	4.459213000	-1.999942000
H	4.624470000	5.153431000	-0.670862000
O	4.934689000	2.099470000	3.682227000
H	4.945097000	1.800712000	2.783474000
H	4.095679000	2.525603000	3.788444000
coord_5			
C	3.198740000	-0.917595000	0.204335000
C	3.122149000	0.498772000	-0.008243000
C	1.933409000	1.153112000	-0.202842000
C	0.809650000	-0.977344000	-0.068794000
C	1.974362000	-1.646287000	0.104914000
C	4.532152000	-1.375359000	0.370287000
C	5.462559000	-0.379801000	0.299629000
N	0.721185000	0.426608000	-0.044928000
H	-0.120661000	-1.495788000	-0.182070000
H	1.966270000	-2.719350000	0.135345000
H	4.788750000	-2.404657000	0.533865000
H	6.523941000	-0.467805000	0.399966000
S	1.861866000	2.876174000	-0.567546000
S	4.744290000	1.205226000	0.012799000

C	-0.586870000	1.067099000	0.108195000
O	-1.381160000	0.870626000	-1.066939000
C	-1.405714000	0.541190000	1.264446000
H	-0.482118000	2.143740000	0.241701000
C	-2.758059000	0.819814000	-0.666140000
C	-2.775869000	0.973353000	0.845315000
H	-1.099191000	0.958899000	2.227326000
H	-1.371838000	-0.547805000	1.352116000
H	-3.267588000	1.675305000	-1.115919000
H	-2.903785000	2.029425000	1.098109000
C	-3.403550000	-0.452449000	-1.212382000
H	-4.476925000	-0.457407000	-1.007807000
H	-3.256402000	-0.520578000	-2.293375000
O	-2.841780000	-1.625329000	-0.636147000
H	-2.818843000	-1.475464000	0.324079000
O	-3.803981000	0.230068000	1.486771000
H	-3.607696000	0.252720000	2.438559000
O	3.929815000	5.152872000	-1.421530000
H	4.251879000	4.475265000	-1.999824000
H	4.544469000	5.277643000	-0.711647000
O	4.941260000	2.128710000	3.677212000
H	4.948690000	1.819254000	2.782222000
H	4.105943000	2.563087000	3.779049000
coord_6			
C	3.192989000	-0.944747000	0.204311000
C	3.124331000	0.476691000	-0.000715000
C	1.940058000	1.138450000	-0.197032000
C	0.804521000	-0.986940000	-0.079130000
C	1.966134000	-1.663625000	0.096194000
C	4.522736000	-1.408790000	0.375418000
C	5.458019000	-0.416430000	0.316296000
N	0.725101000	0.416069000	-0.052728000
H	-0.128166000	-1.500044000	-0.196173000
H	1.950432000	-2.736717000	0.123740000
H	4.774380000	-2.439986000	0.534327000
H	6.518390000	-0.510105000	0.421952000
S	1.885752000	2.858362000	-0.558259000
S	4.749779000	1.174658000	0.033115000
C	-0.580158000	1.062713000	0.097865000
O	-1.375388000	0.864923000	-1.076334000
C	-1.400169000	0.543752000	1.256183000
H	-0.4711477000	2.139507000	0.227443000

C	-2.752308000	0.819434000	-0.675183000
C	-2.768995000	0.978023000	0.835765000
H	-1.092152000	0.964083000	2.217530000
H	-1.369283000	-0.545122000	1.347027000
H	-3.259132000	1.675167000	-1.127549000
H	-2.893887000	2.035302000	1.084766000
C	-3.401813000	-0.452513000	-1.217273000
H	-4.475275000	-0.452791000	-1.013084000
H	-3.254658000	-0.525069000	-2.298005000
O	-2.844522000	-1.625592000	-0.636986000
H	-2.820674000	-1.472806000	0.322752000
O	-3.798755000	0.239545000	1.480391000
H	-3.602285000	0.265717000	2.431951000
O	3.900501000	5.241348000	-1.503845000
H	4.232945000	4.499736000	-1.990460000
H	4.460269000	5.401314000	-0.756602000
O	4.947831000	2.157950000	3.672197000
H	4.952282000	1.837796000	2.780970000
H	4.116301000	2.600523000	3.769641000
coord_7			
C	3.187239000	-0.971898000	0.204288000
C	3.126512000	0.454611000	0.006813000
C	1.946707000	1.123787000	-0.191222000
C	0.799393000	-0.996537000	-0.089465000
C	1.957906000	-1.680962000	0.087473000
C	4.513320000	-1.442221000	0.380549000
C	5.453479000	-0.453059000	0.332963000
N	0.729017000	0.405530000	-0.060528000
H	-0.135553000	-1.504453000	-0.210230000
H	1.934596000	-2.754030000	0.112122000
H	4.760022000	-2.475267000	0.534802000
H	6.512793000	-0.552422000	0.443926000
S	1.909639000	2.840551000	-0.548971000
S	4.755268000	1.144091000	0.053431000
C	-0.574379000	1.058040000	0.090308000
O	-1.371681000	0.860595000	-1.082733000
C	-1.397355000	0.546925000	1.250908000
H	-0.460576000	2.134789000	0.216342000
C	-2.748816000	0.819806000	-0.681160000
C	-2.765679000	0.983419000	0.829154000
H	-1.088769000	0.970456000	2.210667000
H	-1.370054000	-0.541684000	1.346523000

H	-3.252770000	1.675404000	-1.136867000
H	-2.889054000	2.041873000	1.073920000
C	-3.402355000	-0.452216000	-1.218449000
H	-4.475375000	-0.449553000	-1.012197000
H	-3.256809000	-0.528749000	-2.299151000
O	-2.848078000	-1.624622000	-0.634319000
H	-2.822962000	-1.467267000	0.324644000
O	-3.798300000	0.250159000	1.475889000
H	-3.601194000	0.275373000	2.427399000
O	3.871186000	5.329823000	-1.586160000
H	4.209292000	4.535279000	-1.975628000
H	4.372892000	5.523785000	-0.806434000
O	4.954402000	2.187190000	3.667181000
H	4.955875000	1.856338000	2.779719000
H	4.126753000	2.637911000	3.760222000
coord_8			
C	3.181489000	-0.999049000	0.204264000
C	3.128694000	0.432530000	0.014341000
C	1.953356000	1.109125000	-0.185413000
C	0.794265000	-1.006134000	-0.099801000
C	1.949679000	-1.698300000	0.078752000
C	4.503905000	-1.475653000	0.385679000
C	5.448939000	-0.489689000	0.349629000
N	0.732934000	0.394991000	-0.068329000
H	-0.142910000	-1.508857000	-0.224264000
H	1.918808000	-2.771303000	0.100490000
H	4.745864000	-2.510462000	0.535286000
H	6.507151000	-0.594753000	0.465898000
S	1.933525000	2.822739000	-0.539684000
S	4.760757000	1.113524000	0.073746000
C	-0.567082000	1.053668000	0.077737000
O	-1.364836000	0.853762000	-1.094642000
C	-1.390464000	0.548698000	1.240111000
H	-0.449526000	2.130732000	0.198688000
C	-2.741852000	0.818645000	-0.692726000
C	-2.757054000	0.987936000	0.817025000
H	-1.079613000	0.974074000	2.198252000
H	-1.365915000	-0.539696000	1.339330000
H	-3.243993000	1.673938000	-1.150929000
H	-2.875564000	2.047684000	1.058570000
C	-3.399338000	-0.452968000	-1.225846000
H	-4.472806000	-0.445394000	-1.021752000

H	-3.252564000	-0.533690000	-2.306083000
O	-2.849516000	-1.625678000	-0.637698000
H	-2.824457000	-1.466504000	0.320976000
O	-3.791382000	0.260110000	1.466419000
H	-3.594413000	0.290501000	2.417826000
O	3.841872000	5.418299000	-1.668474000
H	4.181064000	4.583138000	-1.959605000
H	4.283516000	5.644474000	-0.861568000
O	4.960974000	2.216431000	3.662166000
H	4.959468000	1.874880000	2.778467000
H	4.137298000	2.675247000	3.750794000
coord_9			
C	3.175738000	-1.026200000	0.204240000
C	3.130876000	0.410450000	0.021869000
C	1.960005000	1.094462000	-0.179603000
C	0.789137000	-1.015731000	-0.110136000
C	1.941451000	-1.715637000	0.070031000
C	4.494489000	-1.509084000	0.390810000
C	5.444400000	-0.526318000	0.366296000
N	0.736850000	0.384452000	-0.076129000
H	-0.150238000	-1.513249000	-0.238285000
H	1.903038000	-2.788531000	0.088849000
H	4.731491000	-2.545672000	0.535751000
H	6.501461000	-0.637099000	0.487861000
S	1.957412000	2.804928000	-0.530397000
S	4.766247000	1.082957000	0.094062000
C	-0.561284000	1.049814000	0.063473000
O	-1.356672000	0.848533000	-1.110511000
C	-1.391115000	0.556151000	1.226596000
H	-0.438837000	2.126808000	0.179134000
C	-2.735109000	0.817136000	-0.713136000
C	-2.755570000	0.995639000	0.795325000
H	-1.083105000	0.988392000	2.182671000
H	-1.369344000	-0.531432000	1.334785000
H	-3.235258000	1.669419000	-1.179219000
H	-2.873568000	2.057109000	1.029375000
C	-3.391256000	-0.457863000	-1.239877000
H	-4.465531000	-0.447280000	-1.040485000
H	-3.239757000	-0.547156000	-2.318790000
O	-2.845793000	-1.626255000	-0.639392000
H	-2.824339000	-1.458766000	0.317978000
O	-3.794229000	0.274220000	1.445431000

H	-3.599940000	0.308221000	2.397197000
O	3.812557000	5.506775000	-1.750789000
H	4.148877000	4.643087000	-1.946322000
H	4.193363000	5.762922000	-0.922129000
O	4.967545000	2.245671000	3.657151000
H	4.963060000	1.893422000	2.777215000
H	4.147934000	2.712528000	3.741357000
coord_10			
C	3.169987900	-1.053351700	0.204216300
C	3.133057700	0.388369400	0.029396700
C	1.966653900	1.079800200	-0.173793000
C	0.784008500	-1.025327900	-0.120471500
C	1.933222800	-1.732974700	0.061310600
C	4.485072700	-1.542514500	0.395940900
C	5.439860000	-0.562947000	0.382962400
N	0.740766100	0.373912700	-0.083929600
H	-0.157611600	-1.517576100	-0.251990500
H	1.887493000	-2.805708700	0.078010000
H	4.717501200	-2.580791400	0.535978500
H	6.495717900	-0.679486300	0.509911700
S	1.981298500	2.787116200	-0.521109600
S	4.771735800	1.052389300	0.114377900
C	-0.555248300	1.044586700	0.051685800
O	-1.351393200	0.840024200	-1.121511500
C	-1.387072000	0.559629100	1.217102300
H	-0.428934700	2.121610900	0.161320800
C	-2.729977000	0.813642400	-0.724258100
C	-2.750591100	0.999732900	0.783270300
H	-1.078565800	0.996283400	2.171071200
H	-1.367640700	-0.527440000	1.331223800
H	-3.228068600	1.664788500	-1.194832700
H	-2.866812000	2.062544800	1.011947800
C	-3.389360900	-0.462404100	-1.244895900
H	-4.463617600	-0.447892600	-1.045958300
H	-3.237658200	-0.557564700	-2.323212500
O	-2.847522500	-1.629271100	-0.638323600
H	-2.825782000	-1.457112100	0.318245800
O	-3.790938000	0.283444800	1.436555900
H	-3.597278700	0.321868500	2.388266700
O	3.783242600	5.595250200	-1.833103700
H	4.113609100	4.713816400	-1.938746000
H	4.103566800	5.878801100	-0.988019300

O	4.974116100	2.274911000	3.652135400
H	4.966652700	1.911963900	2.775963700
H	4.158744600	2.749702800	3.731904600
${}^3\eta\pi^*/{}^3\pi\pi^*$ to $T_1({}^3\pi\pi^*)$ minimum			
coord_1			
C	3.221740900	-0.808990200	0.204430100
C	3.113421900	0.587094200	-0.038355000
C	1.906813500	1.211761300	-0.226081100
C	0.830162200	-0.938956300	-0.027452000
C	2.007273600	-1.576937400	0.139797000
C	4.569816300	-1.241635300	0.349764100
C	5.480717500	-0.233284100	0.232963100
N	0.705520200	0.468764100	-0.013726000
H	-0.091794000	-1.475311400	-0.126363000
H	2.028600600	-2.649344700	0.181429100
H	4.847699400	-2.262269600	0.531686100
H	6.545794800	-0.296667100	0.311845100
S	1.766319500	2.947419800	-0.604695200
S	4.722333300	1.327494400	-0.068464000
C	-0.608287200	1.089436300	0.159376000
O	-1.398754400	0.918012300	-1.021238300
C	-1.423850400	0.530180100	1.302531400
H	-0.511207100	2.162202600	0.322662100
C	-2.775156800	0.845536200	-0.623356200
C	-2.795919800	0.964284300	0.891388200
H	-1.121529300	0.926898300	2.275858600
H	-1.383630400	-0.560095200	1.364226400
H	-3.291707900	1.705832500	-1.055573300
H	-2.930720800	2.013612600	1.167662300
C	-3.405353000	-0.421058100	-1.198545300
H	-4.478988300	-0.441126100	-0.996703300
H	-3.254967900	-0.463751100	-2.280472600
O	-2.832308800	-1.600333400	-0.646499200
H	-2.812528800	-1.471213400	0.316828100
O	-3.820591100	0.200772100	1.514288400
H	-3.622925000	0.198681100	2.466089700
O	4.047073100	4.798969300	-1.092271300
H	4.295292200	4.425816200	-1.928017500
H	4.834617400	4.784014300	-0.562816200
O	4.914975400	2.011749600	3.697273000
H	4.934319400	1.745086500	2.787228800
H	4.064828100	2.413207700	3.816627100

coord_2

C	3.215991000	-0.836141000	0.204406000
C	3.115604000	0.565014000	-0.030827000
C	1.913463000	1.197099000	-0.220271000
C	0.825034000	-0.948553000	-0.037788000
C	1.999046000	-1.594275000	0.131076000
C	4.560400000	-1.275066000	0.354895000
C	5.476178000	-0.269913000	0.249630000
N	0.709436000	0.458225000	-0.021526000
H	-0.098159000	-1.482453000	-0.139875000
H	2.013906000	-2.666967000	0.170084000
H	4.831771000	-2.298445000	0.532526000
H	6.540320000	-0.341001000	0.333988000
S	1.790206000	2.929608000	-0.595408000
S	4.727823000	1.296927000	-0.048148000
C	-0.606628000	1.079650000	0.134167000
O	-1.396570000	0.876601000	-1.042297000
C	-1.419917000	0.539227000	1.287451000
H	-0.515317000	2.156679000	0.273167000
C	-2.773276000	0.810061000	-0.643408000
C	-2.794466000	0.957144000	0.868799000
H	-1.119006000	0.956115000	2.252523000
H	-1.374327000	-0.549705000	1.369552000
H	-3.290219000	1.662443000	-1.090581000
H	-2.935084000	2.010713000	1.125002000
C	-3.404344000	-0.466822000	-1.195150000
H	-4.477588000	-0.484125000	-0.990658000
H	-3.255447000	-0.529049000	-2.276357000
O	-2.830210000	-1.635516000	-0.622657000
H	-2.808215000	-1.487964000	0.337938000
O	-3.813914000	0.199511000	1.507467000
H	-3.619731000	0.223799000	2.459632000
O	4.017759000	4.887445000	-1.174586000
H	4.286919000	4.438094000	-1.963850000
H	4.769098000	4.906046000	-0.598006000
O	4.921547000	2.040990000	3.692258000
H	4.937912000	1.763628000	2.785977000
H	4.075263000	2.450596000	3.807214000

coord_3

C	3.210240000	-0.863293000	0.204382000
C	3.117785000	0.542933000	-0.023299000
C	1.920111000	1.182437000	-0.214461000

C	0.819906000	-0.958150000	-0.048123000
C	1.990818000	-1.611612000	0.122356000
C	4.550984000	-1.308497000	0.360026000
C	5.471638000	-0.306542000	0.266296000
N	0.713353000	0.447686000	-0.029327000
H	-0.105685000	-1.486934000	-0.153948000
H	1.998014000	-2.684474000	0.158525000
H	4.817373000	-2.333901000	0.532995000
H	6.534905000	-0.383252000	0.355985000
S	1.814093000	2.911797000	-0.586121000
S	4.733312000	1.266360000	-0.027832000
C	-0.599233000	1.076390000	0.130422000
O	-1.390405000	0.885000000	-1.046980000
C	-1.416371000	0.536458000	1.281864000
H	-0.501450000	2.152283000	0.274229000
C	-2.767532000	0.825773000	-0.648555000
C	-2.787878000	0.966260000	0.864260000
H	-1.113536000	0.946927000	2.249154000
H	-1.378433000	-0.553073000	1.359744000
H	-3.279738000	1.682608000	-1.092820000
H	-2.921228000	2.019416000	1.125838000
C	-3.406195000	-0.445183000	-1.204784000
H	-4.479535000	-0.456572000	-1.000433000
H	-3.258352000	-0.504695000	-2.286199000
O	-2.838472000	-1.619005000	-0.636062000
H	-2.817559000	-1.475422000	0.325126000
O	-3.813486000	0.212541000	1.497740000
H	-3.615316000	0.222136000	2.449245000
O	3.988444000	4.975921000	-1.256901000
H	4.277817000	4.448044000	-1.988277000
H	4.699503000	5.029355000	-0.633329000
O	4.928118000	2.070230000	3.687242000
H	4.941505000	1.782170000	2.784725000
H	4.085512000	2.488077000	3.797824000

coord_4

C	3.204490000	-0.890444000	0.204359000
C	3.119967000	0.520853000	-0.015771000
C	1.926760000	1.167774000	-0.208652000
C	0.814778000	-0.967747000	-0.058458000
C	1.982590000	-1.628950000	0.113635000
C	4.541568000	-1.341928000	0.365156000
C	5.467098000	-0.343172000	0.282963000

N	0.717269000	0.437147000	-0.037127000
H	-0.113186000	-1.491377000	-0.168010000
H	1.982129000	-2.701940000	0.146942000
H	4.803121000	-2.369290000	0.533383000
H	6.529445000	-0.425514000	0.377975000
S	1.837979000	2.893985000	-0.576833000
S	4.738801000	1.235793000	-0.007517000
C	-0.592830000	1.072158000	0.119835000
O	-1.384974000	0.880048000	-1.057123000
C	-1.412069000	0.538709000	1.272764000
H	-0.490853000	2.148281000	0.259487000
C	-2.762216000	0.825061000	-0.658438000
C	-2.782319000	0.970075000	0.853906000
H	-1.108933000	0.952300000	2.238590000
H	-1.377079000	-0.550702000	1.355106000
H	-3.272006000	1.682022000	-1.105197000
H	-2.912847000	2.024328000	1.112261000
C	-3.404313000	-0.446208000	-1.210383000
H	-4.477751000	-0.453965000	-1.006440000
H	-3.256409000	-0.509627000	-2.291603000
O	-2.840578000	-1.619922000	-0.637495000
H	-2.818688000	-1.473236000	0.323364000
O	-3.809273000	0.221097000	1.490739000
H	-3.610745000	0.234878000	2.442123000
O	3.959130000	5.064396000	-1.339215000
H	4.266530000	4.459213000	-1.999942000
H	4.624470000	5.153431000	-0.670862000
O	4.934689000	2.099470000	3.682227000
H	4.945097000	1.800712000	2.783474000
H	4.095679000	2.525603000	3.788444000
coord_5			
C	3.198740000	-0.917595000	0.204335000
C	3.122149000	0.498772000	-0.008243000
C	1.933409000	1.153112000	-0.202842000
C	0.809650000	-0.977344000	-0.068794000
C	1.974362000	-1.646287000	0.104914000
C	4.532152000	-1.375359000	0.370287000
C	5.462559000	-0.379801000	0.299629000
N	0.721185000	0.426608000	-0.044928000
H	-0.120661000	-1.495788000	-0.182070000
H	1.966270000	-2.719350000	0.135345000
H	4.788750000	-2.404657000	0.533865000

H	6.523941000	-0.467805000	0.399966000
S	1.861866000	2.876174000	-0.567546000
S	4.744290000	1.205226000	0.012799000
C	-0.586870000	1.067099000	0.108195000
O	-1.381160000	0.870626000	-1.066939000
C	-1.405714000	0.541190000	1.264446000
H	-0.482118000	2.143740000	0.241701000
C	-2.758059000	0.819814000	-0.666140000
C	-2.775869000	0.973353000	0.845315000
H	-1.099191000	0.958899000	2.227326000
H	-1.371838000	-0.547805000	1.352116000
H	-3.267588000	1.675305000	-1.115919000
H	-2.903785000	2.029425000	1.098109000
C	-3.403550000	-0.452449000	-1.212382000
H	-4.476925000	-0.457407000	-1.007807000
H	-3.256402000	-0.520578000	-2.293375000
O	-2.841780000	-1.625329000	-0.636147000
H	-2.818843000	-1.475464000	0.324079000
O	-3.803981000	0.230068000	1.486771000
H	-3.607696000	0.252720000	2.438559000
O	3.929815000	5.152872000	-1.421530000
H	4.251879000	4.475265000	-1.999824000
H	4.544469000	5.277643000	-0.711647000
O	4.941260000	2.128710000	3.677212000
H	4.948690000	1.819254000	2.782222000
H	4.105943000	2.563087000	3.779049000

coord_6

C	3.192989000	-0.944747000	0.204311000
C	3.124331000	0.476691000	-0.000715000
C	1.940058000	1.138450000	-0.197032000
C	0.804521000	-0.986940000	-0.079130000
C	1.966134000	-1.663625000	0.096194000
C	4.522736000	-1.408790000	0.375418000
C	5.458019000	-0.416430000	0.316296000
N	0.725101000	0.416069000	-0.052728000
H	-0.128166000	-1.500044000	-0.196173000
H	1.950432000	-2.736717000	0.123740000
H	4.774380000	-2.439986000	0.534327000
H	6.518390000	-0.510105000	0.421952000
S	1.885752000	2.858362000	-0.558259000
S	4.749779000	1.174658000	0.033115000
C	-0.580158000	1.062713000	0.097865000

O	-1.375388000	0.864923000	-1.076334000
C	-1.400169000	0.543752000	1.256183000
H	-0.471477000	2.139507000	0.227443000
C	-2.752308000	0.819434000	-0.675183000
C	-2.768995000	0.978023000	0.835765000
H	-1.092152000	0.964083000	2.217530000
H	-1.369283000	-0.545122000	1.347027000
H	-3.259132000	1.675167000	-1.127549000
H	-2.893887000	2.035302000	1.084766000
C	-3.401813000	-0.452513000	-1.217273000
H	-4.475275000	-0.452791000	-1.013084000
H	-3.254658000	-0.525069000	-2.298005000
O	-2.844522000	-1.625592000	-0.636986000
H	-2.820674000	-1.472806000	0.322752000
O	-3.798755000	0.239545000	1.480391000
H	-3.602285000	0.265717000	2.431951000
O	3.900501000	5.241348000	-1.503845000
H	4.232945000	4.499736000	-1.990460000
H	4.460269000	5.401314000	-0.756602000
O	4.947831000	2.157950000	3.672197000
H	4.952282000	1.837796000	2.780970000
H	4.116301000	2.600523000	3.769641000
coord_7			
C	3.187239000	-0.971898000	0.204288000
C	3.126512000	0.454611000	0.006813000
C	1.946707000	1.123787000	-0.191222000
C	0.799393000	-0.996537000	-0.089465000
C	1.957906000	-1.680962000	0.087473000
C	4.513320000	-1.442221000	0.380549000
C	5.453479000	-0.453059000	0.332963000
N	0.729017000	0.405530000	-0.060528000
H	-0.135553000	-1.504453000	-0.210230000
H	1.934596000	-2.754030000	0.112122000
H	4.760022000	-2.475267000	0.534802000
H	6.512793000	-0.552422000	0.443926000
S	1.909639000	2.840551000	-0.548971000
S	4.755268000	1.144091000	0.053431000
C	-0.574379000	1.058040000	0.090308000
O	-1.371681000	0.860595000	-1.082733000
C	-1.397355000	0.546925000	1.250908000
H	-0.460576000	2.134789000	0.216342000
C	-2.748816000	0.819806000	-0.681160000

C	-2.765679000	0.983419000	0.829154000
H	-1.088769000	0.970456000	2.210667000
H	-1.370054000	-0.541684000	1.346523000
H	-3.252770000	1.675404000	-1.136867000
H	-2.889054000	2.041873000	1.073920000
C	-3.402355000	-0.452216000	-1.218449000
H	-4.475375000	-0.449553000	-1.012197000
H	-3.256809000	-0.528749000	-2.299151000
O	-2.848078000	-1.624622000	-0.634319000
H	-2.822962000	-1.467267000	0.324644000
O	-3.798300000	0.250159000	1.475889000
H	-3.601194000	0.275373000	2.427399000
O	3.871186000	5.329823000	-1.586160000
H	4.209292000	4.535279000	-1.975628000
H	4.372892000	5.523785000	-0.806434000
O	4.954402000	2.187190000	3.667181000
H	4.955875000	1.856338000	2.779719000
H	4.126753000	2.637911000	3.760222000
coord_8			
C	3.181489000	-0.999049000	0.204264000
C	3.128694000	0.432530000	0.014341000
C	1.953356000	1.109125000	-0.185413000
C	0.794265000	-1.006134000	-0.099801000
C	1.949679000	-1.698300000	0.078752000
C	4.503905000	-1.475653000	0.385679000
C	5.448939000	-0.489689000	0.349629000
N	0.732934000	0.394991000	-0.068329000
H	-0.142910000	-1.508857000	-0.224264000
H	1.918808000	-2.771303000	0.100490000
H	4.745864000	-2.510462000	0.535286000
H	6.507151000	-0.594753000	0.465898000
S	1.933525000	2.822739000	-0.539684000
S	4.760757000	1.113524000	0.073746000
C	-0.567082000	1.053668000	0.077737000
O	-1.364836000	0.853762000	-1.094642000
C	-1.390464000	0.548698000	1.240111000
H	-0.449526000	2.130732000	0.198688000
C	-2.741852000	0.818645000	-0.692726000
C	-2.757054000	0.987936000	0.817025000
H	-1.079613000	0.974074000	2.198252000
H	-1.365915000	-0.539696000	1.339330000
H	-3.243993000	1.673938000	-1.150929000

H	-2.875564000	2.047684000	1.058570000
C	-3.399338000	-0.452968000	-1.225846000
H	-4.472806000	-0.445394000	-1.021752000
H	-3.252564000	-0.533690000	-2.306083000
O	-2.849516000	-1.625678000	-0.637698000
H	-2.824457000	-1.466504000	0.320976000
O	-3.791382000	0.260110000	1.466419000
H	-3.594413000	0.290501000	2.417826000
O	3.841872000	5.418299000	-1.668474000
H	4.181064000	4.583138000	-1.959605000
H	4.283516000	5.644474000	-0.861568000
O	4.960974000	2.216431000	3.662166000
H	4.959468000	1.874880000	2.778467000
H	4.137298000	2.675247000	3.750794000
coord_9			
C	3.175738000	-1.026200000	0.204240000
C	3.130876000	0.410450000	0.021869000
C	1.960005000	1.094462000	-0.179603000
C	0.789137000	-1.015731000	-0.110136000
C	1.941451000	-1.715637000	0.070031000
C	4.494489000	-1.509084000	0.390810000
C	5.444400000	-0.526318000	0.366296000
N	0.736850000	0.384452000	-0.076129000
H	-0.150238000	-1.513249000	-0.238285000
H	1.903038000	-2.788531000	0.088849000
H	4.731491000	-2.545672000	0.535751000
H	6.501461000	-0.637099000	0.487861000
S	1.957412000	2.804928000	-0.530397000
S	4.766247000	1.082957000	0.094062000
C	-0.561284000	1.049814000	0.063473000
O	-1.356672000	0.848533000	-1.110511000
C	-1.391115000	0.556151000	1.226596000
H	-0.438837000	2.126808000	0.179134000
C	-2.735109000	0.817136000	-0.713136000
C	-2.755570000	0.995639000	0.795325000
H	-1.083105000	0.988392000	2.182671000
H	-1.369344000	-0.531432000	1.334785000
H	-3.235258000	1.669419000	-1.179219000
H	-2.873568000	2.057109000	1.029375000
C	-3.391256000	-0.457863000	-1.239877000
H	-4.465531000	-0.447280000	-1.040485000
H	-3.239757000	-0.547156000	-2.318790000

O	-2.845793000	-1.626255000	-0.639392000
H	-2.824339000	-1.458766000	0.317978000
O	-3.794229000	0.274220000	1.445431000
H	-3.599940000	0.308221000	2.397197000
O	3.812557000	5.506775000	-1.750789000
H	4.148877000	4.643087000	-1.946322000
H	4.193363000	5.762922000	-0.922129000
O	4.967545000	2.245671000	3.657151000
H	4.963060000	1.893422000	2.777215000
H	4.147934000	2.712528000	3.741357000
coord_10			
C	3.169987900	-1.053351700	0.204216300
C	3.133057700	0.388369400	0.029396700
C	1.966653900	1.079800200	-0.173793000
C	0.784008500	-1.025327900	-0.120471500
C	1.933222800	-1.732974700	0.061310600
C	4.485072700	-1.542514500	0.395940900
C	5.439860000	-0.562947000	0.382962400
N	0.740766100	0.373912700	-0.083929600
H	-0.157611600	-1.517576100	-0.251990500
H	1.887493000	-2.805708700	0.078010000
H	4.717501200	-2.580791400	0.535978500
H	6.495717900	-0.679486300	0.509911700
S	1.981298500	2.787116200	-0.521109600
S	4.771735800	1.052389300	0.114377900
C	-0.555248300	1.044586700	0.051685800
O	-1.351393200	0.840024200	-1.121511500
C	-1.387072000	0.559629100	1.217102300
H	-0.428934700	2.121610900	0.161320800
C	-2.729977000	0.813642400	-0.724258100
C	-2.750591100	0.999732900	0.783270300
H	-1.078565800	0.996283400	2.171071200
H	-1.367640700	-0.527440000	1.331223800
H	-3.228068600	1.664788500	-1.194832700
H	-2.866812000	2.062544800	1.011947800
C	-3.389360900	-0.462404100	-1.244895900
H	-4.463617600	-0.447892600	-1.045958300
H	-3.237658200	-0.557564700	-2.323212500
O	-2.847522500	-1.629271100	-0.638323600
H	-2.825782000	-1.457112100	0.318245800
O	-3.790938000	0.283444800	1.436555900
H	-3.597278700	0.321868500	2.388266700

O	3.783242600	5.595250200	-1.833103700
H	4.113609100	4.713816400	-1.938746000
H	4.103566800	5.878801100	-0.988019300
O	4.974116100	2.274911000	3.652135400
H	4.966652700	1.911963900	2.775963700
H	4.158744600	2.749702800	3.731904600

S₂(¹ππ*) minimum to T₃(³ππ*) minimum

coord_1

C	3.141221000	-1.102899000	0.079226000
C	3.117087000	0.365888000	-0.017711000
C	1.972624000	1.063409000	-0.190414000
C	0.761152000	-1.000704000	-0.230371000
C	1.928584000	-1.747254000	-0.042164000
C	4.464016000	-1.594669000	0.273491000
C	5.402277000	-0.607660000	0.324689000
N	0.764092000	0.371463000	-0.270608000
H	-0.186630000	-1.483157000	-0.345625000
H	1.846139000	-2.817142000	-0.007927000
H	4.705340000	-2.635066000	0.373157000
H	6.455612000	-0.739690000	0.463629000
S	1.921829000	2.841912000	-0.340868000
S	4.760960000	1.031858000	0.131335000
C	-0.551513000	1.034594000	-0.199561000
O	-1.360926000	0.692345000	-1.330905000
C	-1.362116000	0.663215000	1.022064000
H	-0.473911000	2.119295000	-0.214456000
C	-2.734369000	0.731112000	-0.918676000
C	-2.736609000	1.046493000	0.568478000
H	-1.043691000	1.195412000	1.922735000
H	-1.331855000	-0.407022000	1.242887000
H	-3.217855000	1.551266000	-1.454074000
H	-2.865151000	2.123513000	0.706674000
C	-3.422414000	-0.569525000	-1.325484000
H	-4.492744000	-0.521771000	-1.111586000
H	-3.289662000	-0.752532000	-2.395162000
O	-2.885376000	-1.691974000	-0.636374000
H	-2.840290000	-1.442459000	0.302166000
O	-3.757788000	0.377100000	1.297797000
H	-3.547760000	0.496965000	2.239246000
O	3.847065000	5.683179000	-1.940925000
H	3.408607000	4.850621000	-1.830882000
H	4.710638000	5.555861000	-1.572410000

O	4.817912000	2.198328000	3.645998000
H	4.890663000	1.982088000	2.724811000
H	4.036436000	2.729113000	3.714868000
coord_2			
C	3.144360000	-1.096267000	0.077396000
C	3.121884000	0.363301000	-0.017764000
C	1.967657000	1.070006000	-0.192828000
C	0.759682000	-0.997511000	-0.231066000
C	1.931481000	-1.747616000	-0.043004000
C	4.468565000	-1.591309000	0.272160000
C	5.406358000	-0.605449000	0.324516000
N	0.764970000	0.373005000	-0.270744000
H	-0.188294000	-1.479365000	-0.345969000
H	1.851332000	-2.817290000	-0.008774000
H	4.707570000	-2.632262000	0.371303000
H	6.459813000	-0.735886000	0.463885000
S	1.928681000	2.839250000	-0.340830000
S	4.761363000	1.029951000	0.131840000
C	-0.550874000	1.036069000	-0.199990000
O	-1.360506000	0.694180000	-1.331463000
C	-1.361640000	0.664919000	1.021727000
H	-0.472411000	2.120920000	-0.214997000
C	-2.733971000	0.731801000	-0.919036000
C	-2.736369000	1.047243000	0.568070000
H	-1.043528000	1.197615000	1.922207000
H	-1.331017000	-0.405160000	1.243234000
H	-3.218161000	1.551581000	-1.454364000
H	-2.865598000	2.124159000	0.706244000
C	-3.421381000	-0.569250000	-1.325835000
H	-4.491745000	-0.522080000	-1.111937000
H	-3.288597000	-0.752182000	-2.395516000
O	-2.883903000	-1.691493000	-0.636751000
H	-2.840479000	-1.442643000	0.302022000
O	-3.757160000	0.377223000	1.297387000
H	-3.547113000	0.496969000	2.238848000
O	3.847237000	5.683183000	-1.941300000
H	3.406852000	4.851969000	-1.829258000
H	4.710795000	5.554711000	-1.573199000
O	4.815145000	2.199753000	3.647212000
H	4.886976000	1.988850000	2.724947000
H	4.033899000	2.730242000	3.720060000
coord_3			

C	3.147499000	-1.089635000	0.075566000
C	3.126680000	0.360715000	-0.017817000
C	1.962689000	1.076602000	-0.195242000
C	0.758212000	-0.994318000	-0.231760000
C	1.934377000	-1.747978000	-0.043844000
C	4.473113000	-1.587949000	0.270829000
C	5.410437000	-0.603237000	0.324342000
N	0.765849000	0.374547000	-0.270879000
H	-0.189958000	-1.475572000	-0.346313000
H	1.856525000	-2.817438000	-0.009622000
H	4.709798000	-2.629457000	0.369449000
H	6.464013000	-0.732082000	0.464141000
S	1.935532000	2.836587000	-0.340792000
S	4.761765000	1.028043000	0.132345000
C	-0.550235000	1.037543000	-0.200419000
O	-1.360086000	0.696016000	-1.332021000
C	-1.361164000	0.666623000	1.021391000
H	-0.470911000	2.122543000	-0.215538000
C	-2.733571000	0.732491000	-0.919396000
C	-2.736128000	1.047994000	0.567662000
H	-1.043365000	1.199818000	1.921679000
H	-1.330178000	-0.403299000	1.243581000
H	-3.218467000	1.551895000	-1.454653000
H	-2.866044000	2.124803000	0.705813000
C	-3.420347000	-0.568975000	-1.326186000
H	-4.490746000	-0.522389000	-1.112288000
H	-3.287530000	-0.751832000	-2.395870000
O	-2.882430000	-1.691011000	-0.637127000
H	-2.840668000	-1.442826000	0.301878000
O	-3.756532000	0.377346000	1.296977000
H	-3.546465000	0.496974000	2.238449000
O	3.847408000	5.683185000	-1.941675000
H	3.405096000	4.853315000	-1.827634000
H	4.710950000	5.553560000	-1.573987000
O	4.812376000	2.201178000	3.648425000
H	4.883288000	1.995612000	2.725083000
H	4.031361000	2.731370000	3.725250000
coord_4			
C	3.150638000	-1.083004000	0.073737000
C	3.131477000	0.358128000	-0.017871000
C	1.957721000	1.083198000	-0.197656000
C	0.756742000	-0.991125000	-0.232455000

C	1.937273000	-1.748340000	-0.044685000
C	4.477660000	-1.584589000	0.269498000
C	5.414517000	-0.601025000	0.324169000
N	0.766727000	0.376088000	-0.271014000
H	-0.191622000	-1.471779000	-0.346657000
H	1.861717000	-2.817585000	-0.010469000
H	4.712027000	-2.626652000	0.367596000
H	6.468212000	-0.728279000	0.464397000
S	1.942383000	2.833924000	-0.340754000
S	4.762167000	1.026136000	0.132850000
C	-0.549597000	1.039018000	-0.200848000
O	-1.359667000	0.697851000	-1.332578000
C	-1.360688000	0.668327000	1.021054000
H	-0.469411000	2.124167000	-0.216079000
C	-2.733172000	0.733180000	-0.919755000
C	-2.735886000	1.048744000	0.567253000
H	-1.043201000	1.202020000	1.921150000
H	-1.329339000	-0.401437000	1.243929000
H	-3.218773000	1.552210000	-1.454942000
H	-2.866490000	2.125448000	0.705382000
C	-3.419313000	-0.568700000	-1.326537000
H	-4.489746000	-0.522697000	-1.112639000
H	-3.286464000	-0.751481000	-2.396224000
O	-2.880956000	-1.690529000	-0.637504000
H	-2.840857000	-1.443009000	0.301735000
O	-3.755903000	0.377469000	1.296566000
H	-3.545818000	0.496978000	2.238050000
O	3.847578000	5.683187000	-1.942050000
H	3.403340000	4.854661000	-1.826009000
H	4.711106000	5.552409000	-1.574775000
O	4.809607000	2.202603000	3.649639000
H	4.879600000	2.002374000	2.725218000
H	4.028823000	2.732498000	3.730440000
coord_5			
C	3.153776000	-1.076372000	0.071907000
C	3.136273000	0.355542000	-0.017924000
C	1.952753000	1.089795000	-0.200070000
C	0.755272000	-0.987932000	-0.233150000
C	1.940169000	-1.748702000	-0.045525000
C	4.482208000	-1.581229000	0.268167000
C	5.418596000	-0.598814000	0.323995000
N	0.767605000	0.377630000	-0.271150000

H	-0.193286000	-1.467986000	-0.347002000
H	1.866910000	-2.817733000	-0.011317000
H	4.714255000	-2.623847000	0.365742000
H	6.472411000	-0.724475000	0.464653000
S	1.949235000	2.831261000	-0.340715000
S	4.762568000	1.024228000	0.133355000
C	-0.548958000	1.040492000	-0.201277000
O	-1.359247000	0.699686000	-1.333136000
C	-1.360212000	0.670031000	1.020717000
H	-0.467911000	2.125792000	-0.216619000
C	-2.732773000	0.733869000	-0.920115000
C	-2.735645000	1.049494000	0.566845000
H	-1.043038000	1.204223000	1.920622000
H	-1.328500000	-0.399575000	1.244276000
H	-3.219078000	1.552524000	-1.455231000
H	-2.866936000	2.126093000	0.704952000
C	-3.418279000	-0.568424000	-1.326888000
H	-4.488746000	-0.523006000	-1.112990000
H	-3.285397000	-0.751131000	-2.396577000
O	-2.879482000	-1.690048000	-0.637881000
H	-2.841046000	-1.443193000	0.301591000
O	-3.755274000	0.377592000	1.296156000
H	-3.545170000	0.496982000	2.237652000
O	3.847749000	5.683190000	-1.942425000
H	3.401584000	4.856007000	-1.824385000
H	4.711261000	5.551258000	-1.575563000
O	4.806838000	2.204028000	3.650852000
H	4.875913000	2.009135000	2.725354000
H	4.026285000	2.733625000	3.735631000

coord_6

C	3.156915000	-1.069740000	0.070077000
C	3.141069000	0.352955000	-0.017977000
C	1.947785000	1.096391000	-0.202485000
C	0.753802000	-0.984739000	-0.233844000
C	1.943065000	-1.749064000	-0.046365000
C	4.486756000	-1.577869000	0.266836000
C	5.422676000	-0.596602000	0.323822000
N	0.768483000	0.379172000	-0.271285000
H	-0.194951000	-1.464194000	-0.347346000
H	1.872103000	-2.817881000	-0.012164000
H	4.716484000	-2.621043000	0.363888000
H	6.476611000	-0.720671000	0.464909000

S	1.956086000	2.828598000	-0.340677000
S	4.762970000	1.022321000	0.133860000
C	-0.548319000	1.041967000	-0.201706000
O	-1.358827000	0.701522000	-1.333694000
C	-1.359736000	0.671735000	1.020381000
H	-0.466410000	2.127416000	-0.217160000
C	-2.732374000	0.734558000	-0.920475000
C	-2.735404000	1.050244000	0.566437000
H	-1.042874000	1.206426000	1.920093000
H	-1.327661000	-0.397713000	1.244623000
H	-3.219384000	1.552838000	-1.455521000
H	-2.867382000	2.126738000	0.704521000
C	-3.417245000	-0.568149000	-1.327239000
H	-4.487746000	-0.523315000	-1.113340000
H	-3.284331000	-0.750781000	-2.396931000
O	-2.878009000	-1.689566000	-0.638257000
H	-2.841235000	-1.443376000	0.301447000
O	-3.754646000	0.377716000	1.295745000
H	-3.544522000	0.496986000	2.237253000
O	3.847920000	5.683192000	-1.942800000
H	3.399828000	4.857353000	-1.822761000
H	4.711417000	5.550106000	-1.576351000
O	4.804070000	2.205453000	3.652065000
H	4.872225000	2.015897000	2.725489000
H	4.023747000	2.734753000	3.740822000
coord_7			
C	3.160053000	-1.063108000	0.068247000
C	3.145865000	0.350369000	-0.018030000
C	1.942817000	1.102988000	-0.204899000
C	0.752331000	-0.981546000	-0.234539000
C	1.945962000	-1.749426000	-0.047205000
C	4.491303000	-1.574509000	0.265506000
C	5.426755000	-0.594391000	0.323649000
N	0.769361000	0.380714000	-0.271420000
H	-0.196615000	-1.460401000	-0.347690000
H	1.877295000	-2.818028000	-0.013012000
H	4.718712000	-2.618238000	0.362034000
H	6.480810000	-0.716867000	0.465166000
S	1.962937000	2.825935000	-0.340639000
S	4.763372000	1.020413000	0.134365000
C	-0.547680000	1.043441000	-0.202135000
O	-1.358407000	0.703357000	-1.334251000

C	-1.359260000	0.673439000	1.020044000
H	-0.464910000	2.129039000	-0.217701000
C	-2.731975000	0.735248000	-0.920834000
C	-2.735163000	1.050994000	0.566028000
H	-1.042711000	1.208628000	1.919565000
H	-1.326822000	-0.395852000	1.244970000
H	-3.219689000	1.553153000	-1.455810000
H	-2.867828000	2.127383000	0.704090000
C	-3.416211000	-0.567874000	-1.327590000
H	-4.486746000	-0.523623000	-1.113691000
H	-3.283265000	-0.750430000	-2.397285000
O	-2.876535000	-1.689084000	-0.638634000
H	-2.841423000	-1.443559000	0.301303000
O	-3.754017000	0.377839000	1.295335000
H	-3.543874000	0.496990000	2.236854000
O	3.848091000	5.683194000	-1.943174000
H	3.398072000	4.858700000	-1.821136000
H	4.711573000	5.548955000	-1.577140000
O	4.801301000	2.206878000	3.653278000
H	4.868537000	2.022658000	2.725624000
H	4.021209000	2.735881000	3.746012000
coord_8			
C	3.163192000	-1.056476000	0.066418000
C	3.150662000	0.347782000	-0.018083000
C	1.937849000	1.109584000	-0.207313000
C	0.750861000	-0.978353000	-0.235234000
C	1.948858000	-1.749788000	-0.048045000
C	4.495851000	-1.571148000	0.264175000
C	5.430834000	-0.592179000	0.323475000
N	0.770239000	0.382255000	-0.271556000
H	-0.198279000	-1.456608000	-0.348034000
H	1.882488000	-2.818176000	-0.013859000
H	4.720941000	-2.615433000	0.360180000
H	6.485010000	-0.713063000	0.465422000
S	1.969789000	2.823272000	-0.340601000
S	4.763773000	1.018506000	0.134871000
C	-0.547041000	1.044916000	-0.202564000
O	-1.357987000	0.705192000	-1.334809000
C	-1.358784000	0.675144000	1.019707000
H	-0.463410000	2.130663000	-0.218242000
C	-2.731575000	0.735937000	-0.921194000
C	-2.734922000	1.051744000	0.565620000

H	-1.042547000	1.210831000	1.919036000
H	-1.325983000	-0.393990000	1.245317000
H	-3.219995000	1.553467000	-1.456099000
H	-2.868274000	2.128028000	0.703660000
C	-3.415177000	-0.567599000	-1.327941000
H	-4.485747000	-0.523932000	-1.114042000
H	-3.282198000	-0.750080000	-2.397639000
O	-2.875062000	-1.688603000	-0.639011000
H	-2.841612000	-1.443742000	0.301159000
O	-3.753388000	0.377962000	1.294925000
H	-3.543226000	0.496994000	2.236456000
O	3.848262000	5.683197000	-1.943549000
H	3.396316000	4.860046000	-1.819512000
H	4.711728000	5.547804000	-1.577928000
O	4.798532000	2.208303000	3.654491000
H	4.864849000	2.029420000	2.725760000
H	4.018671000	2.737009000	3.751203000
coord_9			
C	3.166330000	-1.049844000	0.064588000
C	3.155458000	0.345195000	-0.018136000
C	1.932881000	1.116180000	-0.209727000
C	0.749391000	-0.975160000	-0.235928000
C	1.951754000	-1.750150000	-0.048886000
C	4.500399000	-1.567788000	0.262844000
C	5.434914000	-0.589967000	0.323302000
N	0.771117000	0.383797000	-0.271691000
H	-0.199943000	-1.452816000	-0.348378000
H	1.887681000	-2.818323000	-0.014707000
H	4.723169000	-2.612628000	0.358326000
H	6.489209000	-0.709259000	0.465678000
S	1.976640000	2.820610000	-0.340563000
S	4.764175000	1.016598000	0.135376000
C	-0.546403000	1.046391000	-0.202993000
O	-1.357567000	0.707028000	-1.335366000
C	-1.358308000	0.676848000	1.019370000
H	-0.461910000	2.132287000	-0.218783000
C	-2.731176000	0.736626000	-0.921554000
C	-2.734681000	1.052495000	0.565211000
H	-1.042384000	1.213034000	1.918508000
H	-1.325145000	-0.392128000	1.245664000
H	-3.220301000	1.553782000	-1.456388000
H	-2.868720000	2.128673000	0.703229000

C	-3.414143000	-0.567324000	-1.328292000
H	-4.484747000	-0.524241000	-1.114393000
H	-3.281132000	-0.749730000	-2.397992000
O	-2.873588000	-1.688121000	-0.639387000
H	-2.841801000	-1.443926000	0.301015000
O	-3.752760000	0.378085000	1.294514000
H	-3.542578000	0.496999000	2.236057000
O	3.848432000	5.683199000	-1.943924000
H	3.394560000	4.861392000	-1.817888000
H	4.711884000	5.546653000	-1.578716000
O	4.795763000	2.209728000	3.655704000
H	4.861161000	2.036182000	2.725895000
H	4.016133000	2.738137000	3.756393000
coord_10			
C	3.169551000	-1.043074000	0.062706000
C	3.160334000	0.342746000	-0.018246000
C	1.927992000	1.122911000	-0.212200000
C	0.748004000	-0.971834000	-0.236676000
C	1.954734000	-1.750376000	-0.049776000
C	4.505029000	-1.564287000	0.261463000
C	5.439074000	-0.587613000	0.323076000
N	0.772076000	0.385471000	-0.271884000
H	-0.201523000	-1.448892000	-0.348774000
H	1.892959000	-2.818335000	-0.015601000
H	4.725482000	-2.609681000	0.356426000
H	6.493489000	-0.705310000	0.465882000
S	1.983567000	2.818080000	-0.340589000
S	4.764655000	1.014831000	0.135823000
C	-0.545684000	1.047995000	-0.203482000
O	-1.357066000	0.708988000	-1.335983000
C	-1.357752000	0.678684000	1.018974000
H	-0.460332000	2.134041000	-0.219387000
C	-2.730696000	0.737439000	-0.921973000
C	-2.734360000	1.053373000	0.564742000
H	-1.042142000	1.215372000	1.917918000
H	-1.324224000	-0.390133000	1.245955000
H	-3.220526000	1.554217000	-1.456740000
H	-2.869088000	2.129446000	0.702734000
C	-3.413025000	-0.566927000	-1.328699000
H	-4.483663000	-0.524429000	-1.114800000
H	-3.279981000	-0.749261000	-2.398401000
O	-2.872029000	-1.687514000	-0.639816000

H	-2.841905000	-1.443981000	0.300818000
O	-3.752050000	0.378337000	1.294044000
H	-3.541850000	0.497135000	2.235598000
O	3.848674000	5.683332000	-1.944371000
H	3.392877000	4.862869000	-1.816333000
H	4.712110000	5.545635000	-1.579576000
O	4.793069000	2.211304000	3.656855000
H	4.857548000	2.043092000	2.725969000
H	4.013669000	2.739415000	3.761519000

S₁(¹nπ*) minimum to T₃(³ππ*) minimum

coord_1

C	3.168011000	-1.042290000	0.103688000
C	3.135127000	0.388565000	0.008919000
C	1.982509000	1.093285000	-0.186874000
C	0.785599000	-1.006763000	-0.250452000
C	1.918243000	-1.722203000	-0.065151000
C	4.475254000	-1.549645000	0.295311000
C	5.440760000	-0.575928000	0.351958000
N	0.757405000	0.394479000	-0.244975000
H	-0.159306000	-1.487760000	-0.400968000
H	1.866132000	-2.794468000	-0.069424000
H	4.699534000	-2.594861000	0.388321000
H	6.493233000	-0.700630000	0.494209000
S	2.016688000	2.860942000	-0.371244000
S	4.774636000	1.045681000	0.166021000
C	-0.545491000	1.062583000	-0.145435000
O	-1.356002000	0.768778000	-1.289194000
C	-1.355847000	0.643970000	1.059857000
H	-0.438018000	2.146366000	-0.116825000
C	-2.729346000	0.776633000	-0.873476000
C	-2.730020000	1.046432000	0.621926000
H	-1.035300000	1.136864000	1.981847000
H	-1.325305000	-0.434989000	1.234662000
H	-3.225280000	1.605742000	-1.383562000
H	-2.854293000	2.119207000	0.792237000
C	-3.403958000	-0.520232000	-1.315883000
H	-4.475674000	-0.487387000	-1.105270000
H	-3.265737000	-0.675123000	-2.389170000
O	-2.860548000	-1.655933000	-0.653993000
H	-2.833341000	-1.435895000	0.292534000
O	-3.753941000	0.359569000	1.330707000
H	-3.556522000	0.470104000	2.276089000

O	3.738933000	5.560078000	-1.919442000
H	3.522234000	4.773062000	-2.406993000
H	4.630857000	5.434901000	-1.624613000
O	4.875585000	2.229663000	3.692187000
H	4.916939000	1.827127000	2.834402000
H	4.044707000	2.684185000	3.711690000
coord_2			
C	3.168251000	-1.042335000	0.099186000
C	3.137992000	0.383517000	0.005962000
C	1.976513000	1.096618000	-0.189621000
C	0.781490000	-1.002845000	-0.248868000
C	1.922369000	-1.725293000	-0.063395000
C	4.478633000	-1.551227000	0.291598000
C	5.440641000	-0.577179000	0.348803000
N	0.759100000	0.393516000	-0.247902000
H	-0.164000000	-1.483375000	-0.395257000
H	1.868882000	-2.797274000	-0.063543000
H	4.702150000	-2.596578000	0.384752000
H	6.493332000	-0.700368000	0.491091000
S	2.013064000	2.856221000	-0.367760000
S	4.773590000	1.042301000	0.162731000
C	-0.545378000	1.060962000	-0.151793000
O	-1.356111000	0.762008000	-1.294330000
C	-1.356053000	0.647860000	1.055364000
H	-0.440508000	2.145062000	-0.128086000
C	-2.729412000	0.772290000	-0.878853000
C	-2.730408000	1.047310000	0.615709000
H	-1.036080000	1.145677000	1.974845000
H	-1.325211000	-0.430043000	1.236050000
H	-3.224725000	1.600023000	-1.391620000
H	-2.855806000	2.120421000	0.782405000
C	-3.404909000	-0.525377000	-1.317286000
H	-4.476475000	-0.491517000	-1.106235000
H	-3.267318000	-0.683262000	-2.390205000
O	-2.861822000	-1.659459000	-0.652387000
H	-2.834215000	-1.436733000	0.293533000
O	-3.753640000	0.361674000	1.326715000
H	-3.554802000	0.473058000	2.271660000
O	3.751174000	5.573831000	-1.922116000
H	3.502597000	4.765824000	-2.350429000
H	4.640248000	5.447218000	-1.619407000
O	4.866478000	2.227647000	3.688334000

H	4.910483000	1.850451000	2.820811000
H	4.040860000	2.690599000	3.717319000
coord_3			
C	3.168491000	-1.042379000	0.094685000
C	3.140858000	0.378470000	0.003005000
C	1.970518000	1.099951000	-0.192368000
C	0.777381000	-0.998927000	-0.247283000
C	1.926494000	-1.728384000	-0.061638000
C	4.482012000	-1.552808000	0.287885000
C	5.440521000	-0.578429000	0.345648000
N	0.760794000	0.392553000	-0.250829000
H	-0.168524000	-1.479399000	-0.389475000
H	1.871556000	-2.800008000	-0.057708000
H	4.705284000	-2.598126000	0.381280000
H	6.493436000	-0.700365000	0.487969000
S	2.009441000	2.851501000	-0.364276000
S	4.772544000	1.038920000	0.159440000
C	-0.545346000	1.059358000	-0.158186000
O	-1.356149000	0.755425000	-1.299490000
C	-1.356200000	0.651746000	1.050884000
H	-0.442908000	2.143752000	-0.139418000
C	-2.729499000	0.767973000	-0.884176000
C	-2.730837000	1.048074000	0.609419000
H	-1.036741000	1.154414000	1.967836000
H	-1.324998000	-0.425080000	1.237352000
H	-3.224129000	1.594356000	-1.399686000
H	-2.857412000	2.121587000	0.772530000
C	-3.405859000	-0.530533000	-1.318635000
H	-4.477305000	-0.495589000	-1.107243000
H	-3.268813000	-0.691479000	-2.391169000
O	-2.863008000	-1.662942000	-0.650766000
H	-2.835098000	-1.437611000	0.294519000
O	-3.753378000	0.363768000	1.322699000
H	-3.553111000	0.476091000	2.267237000
O	3.763415000	5.587584000	-1.924790000
H	3.482225000	4.759675000	-2.290325000
H	4.649568000	5.459544000	-1.614220000
O	4.857370000	2.225631000	3.684481000
H	4.904069000	1.873626000	2.806574000
H	4.036954000	2.697060000	3.722962000
coord_4			
C	3.168731000	-1.042423000	0.090183000

C	3.143723000	0.373422000	0.000048000
C	1.964522000	1.103283000	-0.195115000
C	0.773273000	-0.995008000	-0.245699000
C	1.930620000	-1.731474000	-0.059882000
C	4.485391000	-1.554390000	0.284172000
C	5.440401000	-0.579679000	0.342493000
N	0.762488000	0.391589000	-0.253757000
H	-0.173042000	-1.475413000	-0.383695000
H	1.874261000	-2.802732000	-0.051869000
H	4.708423000	-2.599680000	0.377803000
H	6.493538000	-0.700391000	0.484839000
S	2.005818000	2.846780000	-0.360791000
S	4.771497000	1.035539000	0.156150000
C	-0.545306000	1.057754000	-0.164575000
O	-1.356198000	0.748823000	-1.304639000
C	-1.356352000	0.655630000	1.046404000
H	-0.445320000	2.142434000	-0.150744000
C	-2.729586000	0.763651000	-0.889504000
C	-2.731261000	1.048853000	0.603136000
H	-1.037420000	1.163155000	1.960820000
H	-1.324800000	-0.420106000	1.238664000
H	-3.223536000	1.588678000	-1.407749000
H	-2.859006000	2.122753000	0.762658000
C	-3.406807000	-0.535687000	-1.319990000
H	-4.478130000	-0.499669000	-1.108246000
H	-3.270319000	-0.699684000	-2.392138000
O	-2.864205000	-1.666426000	-0.649143000
H	-2.835980000	-1.438485000	0.295502000
O	-3.753111000	0.365864000	1.318687000
H	-3.551417000	0.479114000	2.262811000
O	3.775655000	5.601337000	-1.927464000
H	3.462525000	4.758086000	-2.225781000
H	4.658816000	5.471881000	-1.609053000
O	4.848262000	2.223615000	3.680628000
H	4.897627000	1.897205000	2.793031000
H	4.033226000	2.703431000	3.728607000
coord_5			
C	3.168971000	-1.042468000	0.085682000
C	3.146588000	0.368374000	-0.002910000
C	1.958527000	1.106616000	-0.197862000
C	0.769164000	-0.991090000	-0.244115000
C	1.934745000	-1.734565000	-0.058126000

C	4.488770000	-1.555971000	0.280459000
C	5.440282000	-0.580930000	0.339337000
N	0.764182000	0.390626000	-0.256684000
H	-0.177545000	-1.471432000	-0.377909000
H	1.876988000	-2.805442000	-0.046028000
H	4.711561000	-2.601232000	0.374322000
H	6.493627000	-0.700485000	0.481744000
S	2.002195000	2.842060000	-0.357307000
S	4.770451000	1.032159000	0.152859000
C	-0.545266000	1.056152000	-0.170964000
O	-1.356249000	0.742222000	-1.309780000
C	-1.356503000	0.659512000	1.041927000
H	-0.447735000	2.141108000	-0.162070000
C	-2.729672000	0.759330000	-0.894833000
C	-2.731683000	1.049635000	0.596853000
H	-1.038103000	1.171893000	1.953794000
H	-1.324607000	-0.415121000	1.239977000
H	-3.222944000	1.582998000	-1.415810000
H	-2.860597000	2.123915000	0.752787000
C	-3.407753000	-0.540840000	-1.321347000
H	-4.478955000	-0.503749000	-1.109249000
H	-3.271828000	-0.707888000	-2.393105000
O	-2.865404000	-1.669907000	-0.647519000
H	-2.836860000	-1.439359000	0.296481000
O	-3.752841000	0.367963000	1.314674000
H	-3.549722000	0.482136000	2.258382000
O	3.787896000	5.615090000	-1.930137000
H	3.444227000	4.761767000	-2.157838000
H	4.667991000	5.484227000	-1.603910000
O	4.839154000	2.221599000	3.676775000
H	4.891151000	1.921127000	2.780214000
H	4.029674000	2.709705000	3.734248000
coord_6			
C	3.169211000	-1.042512000	0.081181000
C	3.149454000	0.363326000	-0.005867000
C	1.952532000	1.109948000	-0.200609000
C	0.765055000	-0.987171000	-0.242530000
C	1.938870000	-1.737656000	-0.056370000
C	4.492149000	-1.557552000	0.276746000
C	5.440162000	-0.582180000	0.336182000
N	0.765877000	0.389663000	-0.259611000
H	-0.182044000	-1.467448000	-0.372119000

H	1.879747000	-2.808144000	-0.040193000
H	4.714700000	-2.602787000	0.370834000
H	6.493721000	-0.700555000	0.478623000
S	1.998571000	2.837339000	-0.353823000
S	4.769404000	1.028778000	0.149569000
C	-0.545227000	1.054551000	-0.177354000
O	-1.356302000	0.735623000	-1.314912000
C	-1.356653000	0.663392000	1.037452000
H	-0.450149000	2.139771000	-0.173397000
C	-2.729759000	0.755008000	-0.900160000
C	-2.732105000	1.050418000	0.590570000
H	-1.038791000	1.180628000	1.946759000
H	-1.324414000	-0.410124000	1.241289000
H	-3.222351000	1.577313000	-1.423870000
H	-2.862189000	2.125073000	0.742916000
C	-3.408697000	-0.545993000	-1.322704000
H	-4.479778000	-0.507830000	-1.110252000
H	-3.273337000	-0.716090000	-2.394070000
O	-2.866606000	-1.673383000	-0.645891000
H	-2.837742000	-1.440234000	0.297455000
O	-3.752568000	0.370063000	1.310662000
H	-3.548029000	0.485156000	2.253953000
O	3.800137000	5.628844000	-1.932811000
H	3.428024000	4.771158000	-2.087805000
H	4.677095000	5.496583000	-1.598792000
O	4.830047000	2.219584000	3.672922000
H	4.884632000	1.945328000	2.768150000
H	4.026294000	2.715878000	3.739879000

coord_7

C	3.169451000	-1.042556000	0.076679000
C	3.152319000	0.358279000	-0.008824000
C	1.946536000	1.113281000	-0.203356000
C	0.760946000	-0.983253000	-0.240946000
C	1.942996000	-1.740746000	-0.054613000
C	4.495527000	-1.559133000	0.273033000
C	5.440042000	-0.583430000	0.333027000
N	0.767571000	0.388700000	-0.262538000
H	-0.186538000	-1.463457000	-0.366330000
H	1.882539000	-2.810836000	-0.034351000
H	4.717834000	-2.604345000	0.367339000
H	6.493812000	-0.700633000	0.475502000
S	1.994948000	2.832619000	-0.350338000

S	4.768358000	1.025398000	0.146278000
C	-0.545191000	1.052953000	-0.183743000
O	-1.356358000	0.729028000	-1.320036000
C	-1.356801000	0.667271000	1.032980000
H	-0.452565000	2.138425000	-0.184726000
C	-2.729848000	0.750685000	-0.905487000
C	-2.732527000	1.051202000	0.584285000
H	-1.039481000	1.189358000	1.939714000
H	-1.324224000	-0.405115000	1.242601000
H	-3.221757000	1.571626000	-1.431928000
H	-2.863779000	2.126225000	0.733045000
C	-3.409639000	-0.551146000	-1.324061000
H	-4.480602000	-0.511910000	-1.111255000
H	-3.274846000	-0.724292000	-2.395030000
O	-2.867807000	-1.676856000	-0.644261000
H	-2.838623000	-1.441110000	0.298425000
O	-3.752295000	0.372165000	1.306650000
H	-3.546335000	0.488176000	2.249522000
O	3.812378000	5.642597000	-1.935485000
H	3.414498000	4.786361000	-2.017148000
H	4.686127000	5.508950000	-1.593701000
O	4.820939000	2.217568000	3.669070000
H	4.878066000	1.969742000	2.756859000
H	4.023084000	2.721944000	3.745493000
coord_8			
C	3.169691000	-1.042601000	0.072178000
C	3.155184000	0.353231000	-0.011781000
C	1.940541000	1.116613000	-0.206103000
C	0.756837000	-0.979335000	-0.239361000
C	1.947121000	-1.743837000	-0.052857000
C	4.498906000	-1.560715000	0.269321000
C	5.439922000	-0.584681000	0.329872000
N	0.769265000	0.387737000	-0.265466000
H	-0.189464000	-1.463642000	-0.362212000
H	1.882085000	-2.814412000	-0.031841000
H	4.722468000	-2.605575000	0.363827000
H	6.494224000	-0.694953000	0.472138000
S	1.991325000	2.827898000	-0.346854000
S	4.767311000	1.022017000	0.142988000
C	-0.545156000	1.051356000	-0.190134000
O	-1.356415000	0.722438000	-1.325151000
C	-1.356949000	0.671149000	1.028511000

H	-0.454981000	2.137071000	-0.196056000
C	-2.729938000	0.746363000	-0.910813000
C	-2.732947000	1.051986000	0.577998000
H	-1.040174000	1.198082000	1.932660000
H	-1.324035000	-0.400094000	1.243911000
H	-3.221161000	1.565936000	-1.439983000
H	-2.865368000	2.127373000	0.723173000
C	-3.410581000	-0.556297000	-1.325418000
H	-4.481425000	-0.515990000	-1.112259000
H	-3.276357000	-0.732492000	-2.395988000
O	-2.869011000	-1.680323000	-0.642628000
H	-2.839505000	-1.441987000	0.299391000
O	-3.752020000	0.374269000	1.302638000
H	-3.544641000	0.491197000	2.245088000
O	3.824619000	5.656350000	-1.938158000
H	3.404061000	4.807137000	-1.947345000
H	4.695091000	5.521328000	-1.588639000
O	4.811831000	2.215552000	3.665217000
H	4.871445000	1.994299000	2.746357000
H	4.020038000	2.727898000	3.751085000
coord_9			
C	3.169930000	-1.042645000	0.067676000
C	3.158050000	0.348183000	-0.014738000
C	1.934546000	1.119946000	-0.208850000
C	0.752728000	-0.975416000	-0.237777000
C	1.951247000	-1.746927000	-0.051101000
C	4.502285000	-1.562296000	0.265607000
C	5.439802000	-0.585931000	0.326717000
N	0.770960000	0.386773000	-0.268393000
H	-0.192729000	-1.461627000	-0.358760000
H	1.884867000	-2.817048000	-0.030013000
H	4.726711000	-2.606912000	0.360045000
H	6.494680000	-0.692950000	0.468911000
S	1.987702000	2.823178000	-0.343370000
S	4.766265000	1.018636000	0.139697000
C	-0.545122000	1.049753000	-0.196528000
O	-1.356477000	0.715847000	-1.330257000
C	-1.357099000	0.675025000	1.024045000
H	-0.457398000	2.135707000	-0.207387000
C	-2.730027000	0.742039000	-0.916145000
C	-2.733367000	1.052771000	0.571714000
H	-1.040868000	1.206801000	1.925597000

H	-1.323851000	-0.395068000	1.245222000
H	-3.220563000	1.560244000	-1.448037000
H	-2.866957000	2.128518000	0.713301000
C	-3.411521000	-0.561446000	-1.326773000
H	-4.482248000	-0.520067000	-1.113262000
H	-3.277867000	-0.740692000	-2.396943000
O	-2.870217000	-1.683787000	-0.640992000
H	-2.840386000	-1.442862000	0.300354000
O	-3.751743000	0.376377000	1.298625000
H	-3.542947000	0.494218000	2.240655000
O	3.836859000	5.670103000	-1.940832000
H	3.396929000	4.832938000	-1.879746000
H	4.703984000	5.533718000	-1.583608000
O	4.802723000	2.213536000	3.661364000
H	4.864763000	2.018931000	2.736654000
H	4.017152000	2.733736000	3.756650000
coord_10			
C	3.169551000	-1.043074000	0.062706000
C	3.160334000	0.342746000	-0.018246000
C	1.927992000	1.122911000	-0.212200000
C	0.748004000	-0.971834000	-0.236676000
C	1.954734000	-1.750376000	-0.049776000
C	4.505029000	-1.564287000	0.261463000
C	5.439074000	-0.587613000	0.323076000
N	0.772076000	0.385471000	-0.271884000
H	-0.201523000	-1.448892000	-0.348774000
H	1.892959000	-2.818335000	-0.015601000
H	4.725482000	-2.609681000	0.356426000
H	6.493489000	-0.705310000	0.465882000
S	1.983567000	2.818080000	-0.340589000
S	4.764655000	1.014831000	0.135823000
C	-0.545684000	1.047995000	-0.203482000
O	-1.357066000	0.708988000	-1.335983000
C	-1.357752000	0.678684000	1.018974000
H	-0.460332000	2.134041000	-0.219387000
C	-2.730696000	0.737439000	-0.921973000
C	-2.734360000	1.053373000	0.564742000
H	-1.042142000	1.215372000	1.917918000
H	-1.324224000	-0.390133000	1.245955000
H	-3.220526000	1.554217000	-1.456740000
H	-2.869088000	2.129446000	0.702734000
C	-3.413025000	-0.566927000	-1.328699000

H	-4.483663000	-0.524429000	-1.114800000
H	-3.279981000	-0.749261000	-2.398401000
O	-2.872029000	-1.687514000	-0.639816000
H	-2.841905000	-1.443981000	0.300818000
O	-3.752050000	0.378337000	1.294044000
H	-3.541850000	0.497135000	2.235598000
O	3.848674000	5.683332000	-1.944371000
H	3.392877000	4.862869000	-1.816333000
H	4.712110000	5.545635000	-1.579576000
O	4.793069000	2.211304000	3.656855000
H	4.857548000	2.043092000	2.725969000
H	4.013669000	2.739415000	3.761519000